

Figure S7. Structural features that were found to be significantly associated with PFAS bioactivity. Shown below are PFAS structures highlighting the Saagar structural features that are listed in Table 3.

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ATOMS

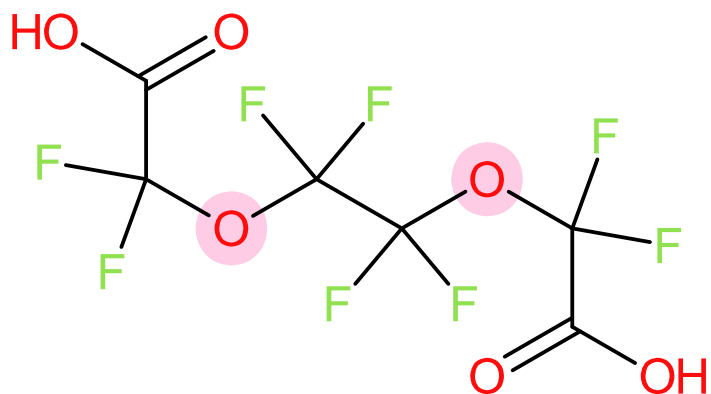
SGR10068 (9 chem)

SGR10032 (3 chem)

SGR10068

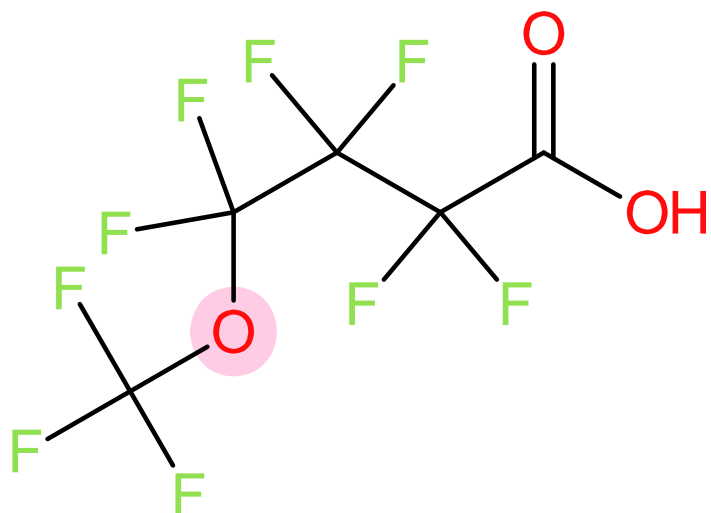
S3: Perfluoro-3,6-dioxaoctane-1,8-dioic acid (PFHx2Et2OA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(O)=O



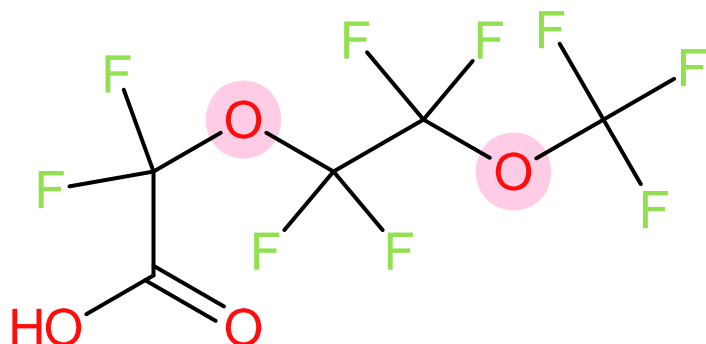
S9: Perfluoro(4-methoxybutanoic) acid (PFMBA)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)F



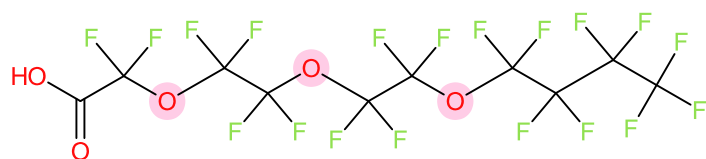
S11: Perfluoro-3,6-dioxaheptanoic acid (NFDHA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



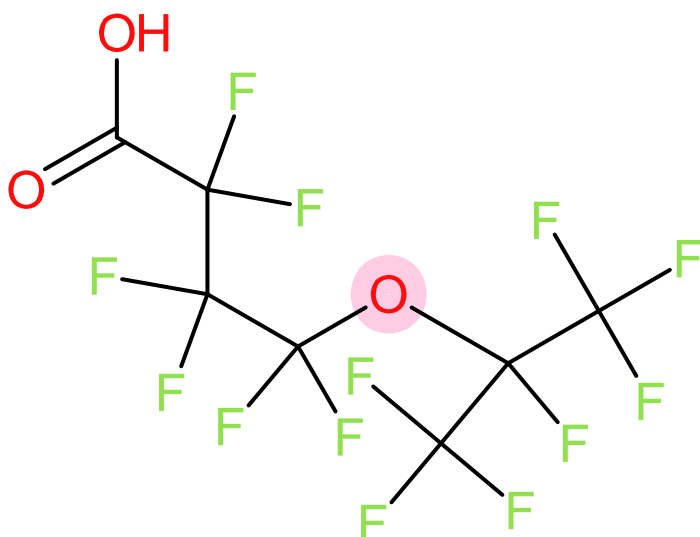
S22: Perfluoro-3,6,9-trioxatridecanoic acid (PFPE-6)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



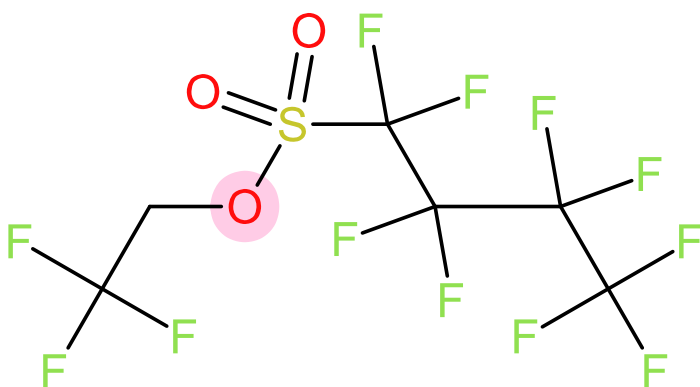
S36: Perfluoro-4-isopropoxybutanoic acid (PFPE-1)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)F



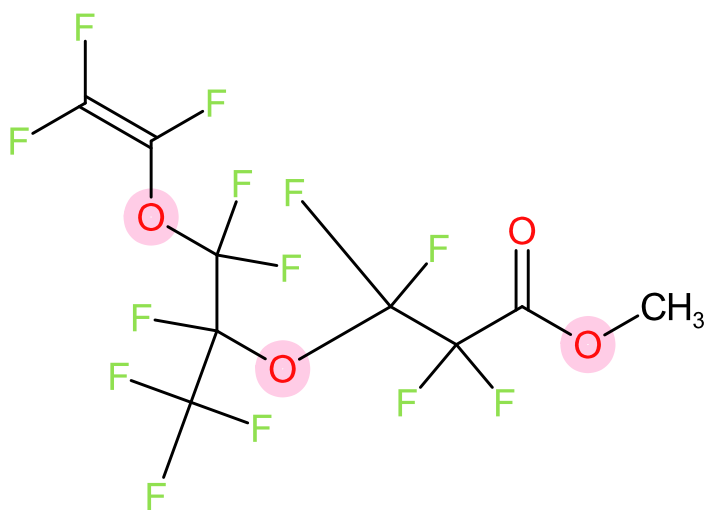
S38: 2,2,2-Trifluoroethyl perfluorobutanesulfonate (ET-PFBS)

SMILES: FC(F)(F)COS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



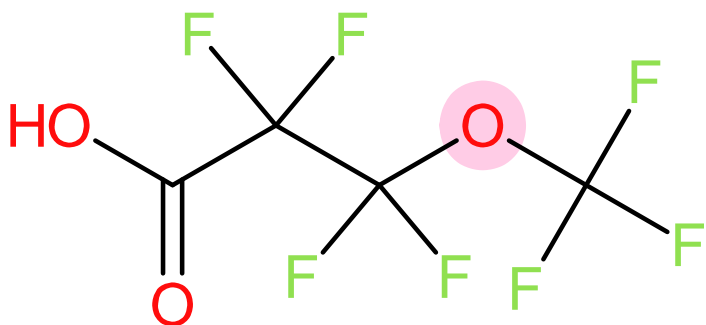
S39: Methyl perfluoro(3-(1-ethenyloxypropan-2-yloxy)propanoate) (MePF2ETOA)

SMILES: COC(=O)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)=C(F)F



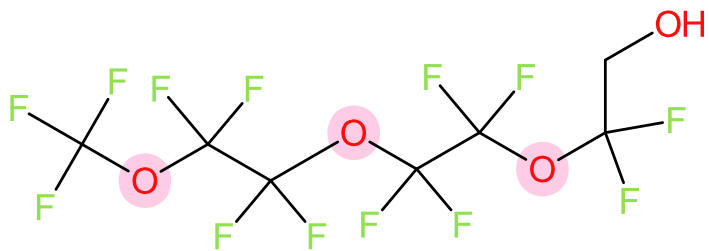
S49: Perfluoro-3-methoxypropanoic acid (PFMPA)

SMILES: OC(=O)C(F)(F)C(F)(F)OC(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

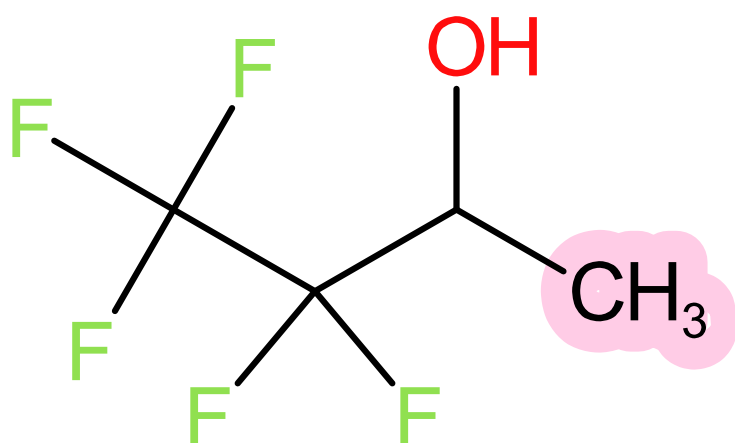
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10032

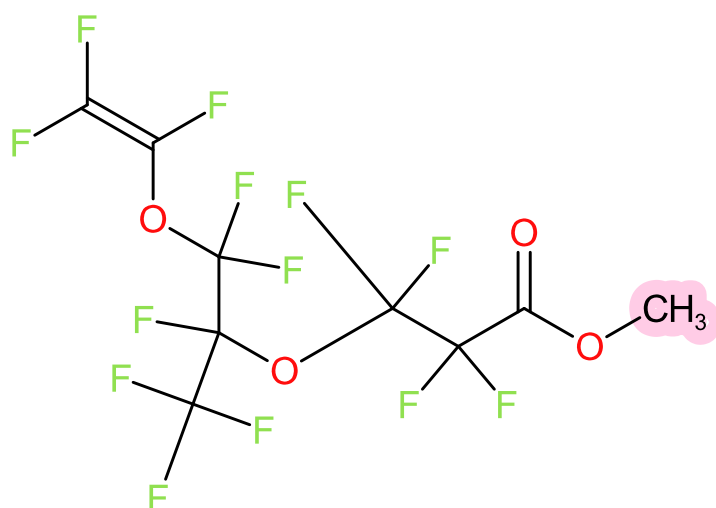
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



S39: Methyl perfluoro(3-(1-ethenyloxypropan-2-yloxy)propanoate) (MePF2ETOA)

SMILES: COC(=O)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)=C(F)F



ATOM PAIRS

SGR10786 (8 chem)

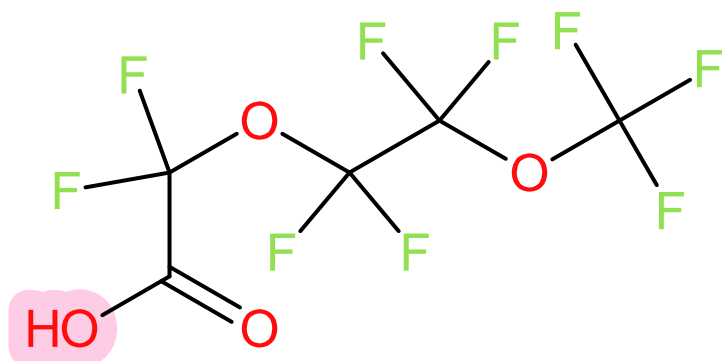
SGR10112 (7 chem)

SGR10199 (3 chem)

SGR10786

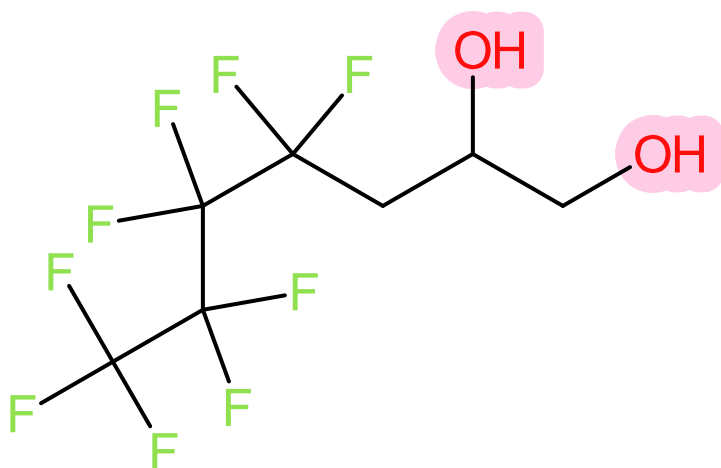
S11: Perfluoro-3,6-dioxaheptanoic acid (NFDHA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



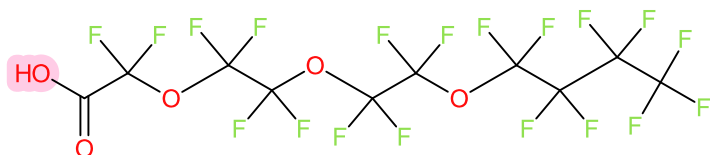
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



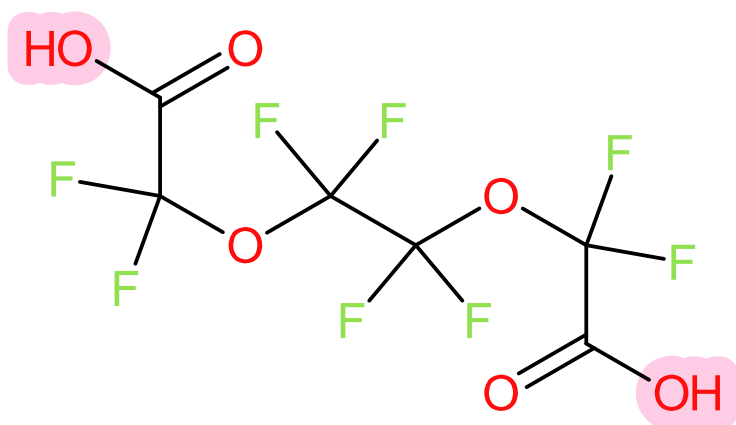
S22: Perfluoro-3,6,9-trioxatridecanoic acid (PFPE-6)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



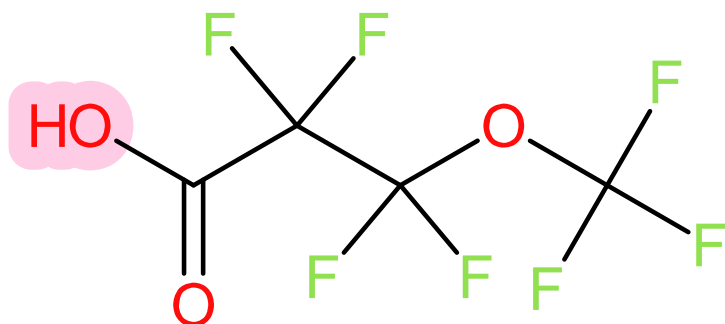
S3: Perfluoro-3,6-dioxaoctane-1,8-dioic acid (PFHx2Et2OA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(O)=O



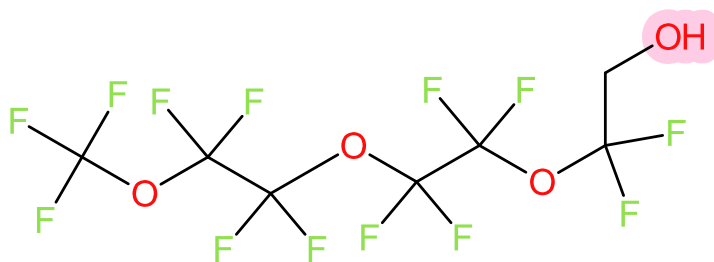
S49: Perfluoro-3-methoxypropanoic acid (PFMPA)

SMILES: OC(=O)C(F)(F)C(F)(F)OC(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C₇F₃ETOH)

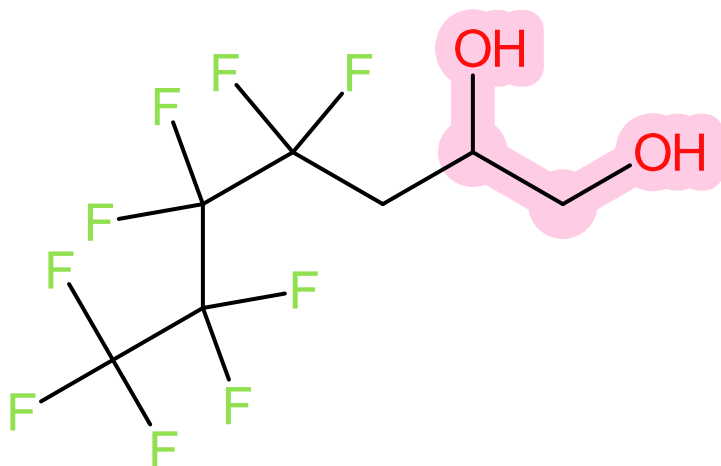
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10112

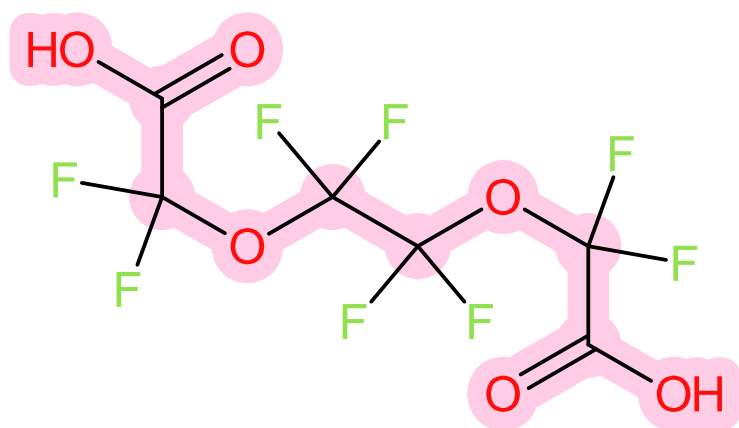
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



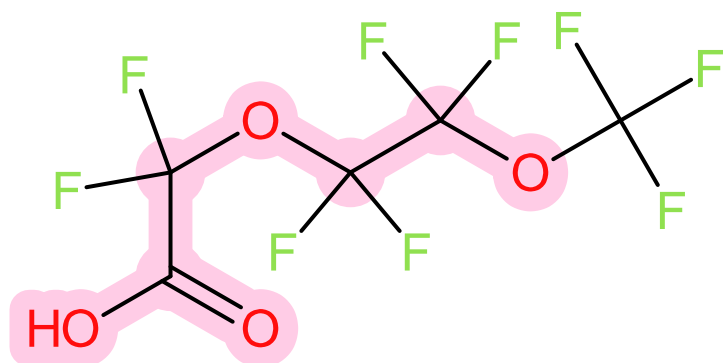
S3: Perfluoro-3,6-dioxaoctane-1,8-dioic acid (PFHx2EtOA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(O)=O



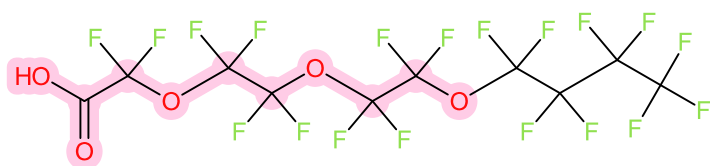
S11: Perfluoro-3,6-dioxaheptanoic acid (NFDHA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



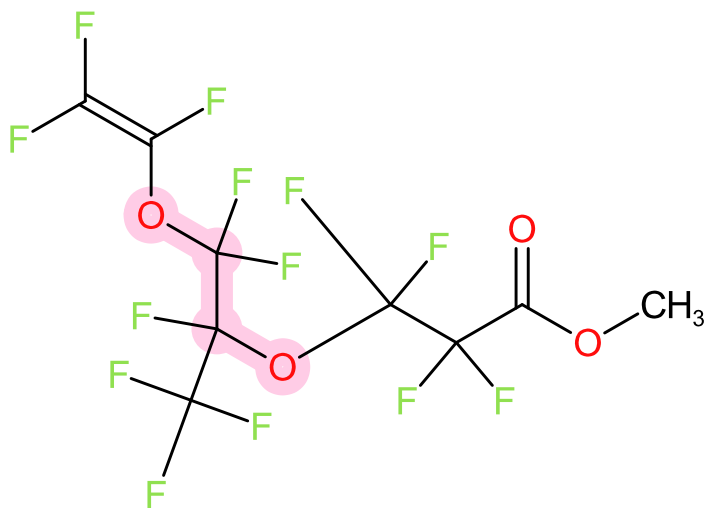
S22: Perfluoro-3,6,9-trioxatridecanoic acid (PFPE-6)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



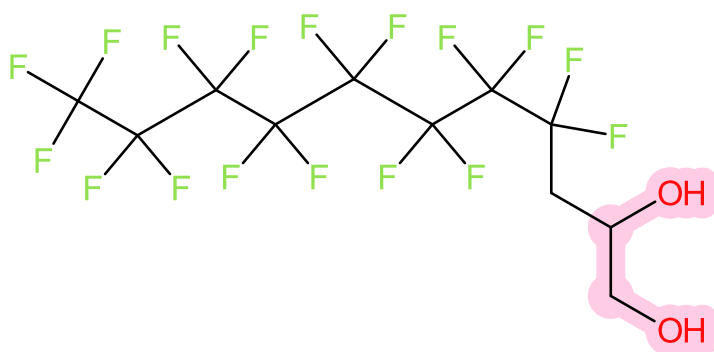
S39: Methyl perfluoro(3-(1-ethenyloxypropan-2-yloxy)propanoate) (MePF2ETOA)

SMILES: COC(=O)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)=C(F)F



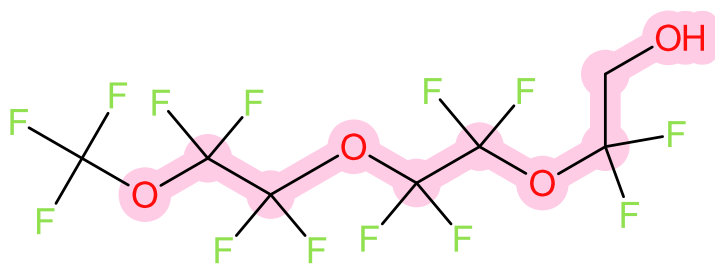
S40: 1-(Perfluorooctyl)propane-2,3-diol (PFUd2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

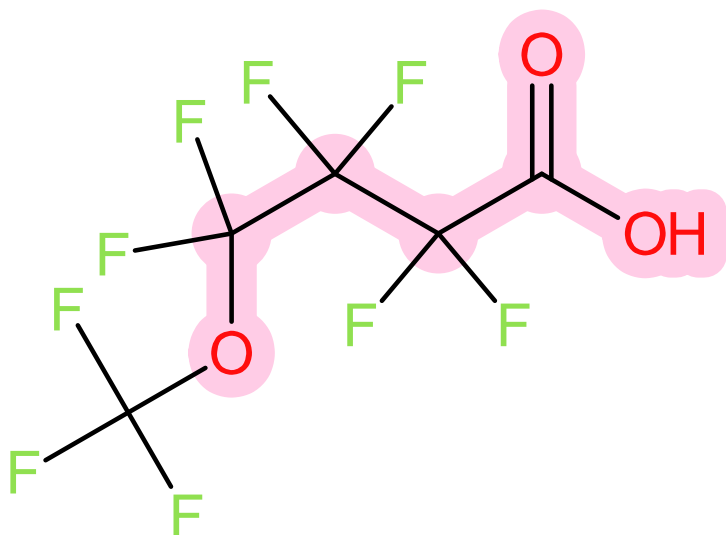
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10199

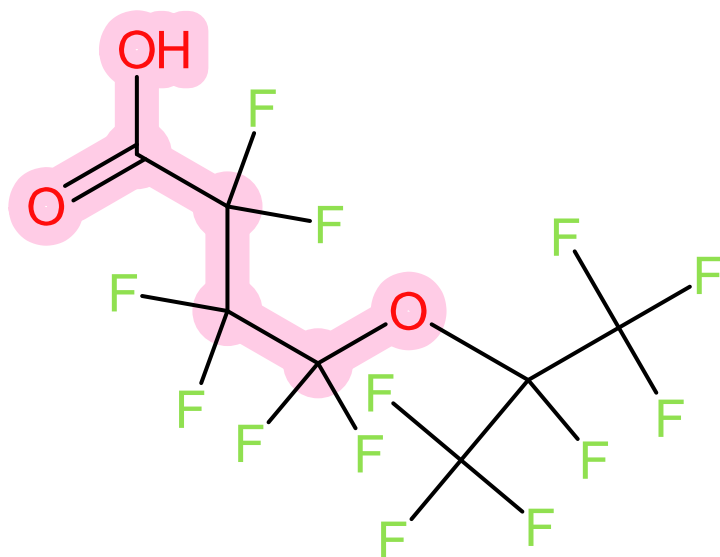
S9: Perfluoro(4-methoxybutanoic) acid (PFMBA)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)F



S36: Perfluoro-4-isopropoxybutanoic acid (PFPE-1)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)F



BIOAVAILIBILITY

SGR10633 (17 chem)

SGR10708 (17 chem)

SGR10275 (12 chem)

SGR10169 (8 chem)

SGR10795 (4 chem)

SGR10290 (3 chem)

SGR10418 (3 chem)

SGR10493 (3 chem)

SGR10684 (3 chem)

SGR10736 (3 chem)

SGR10354 (2 chem)

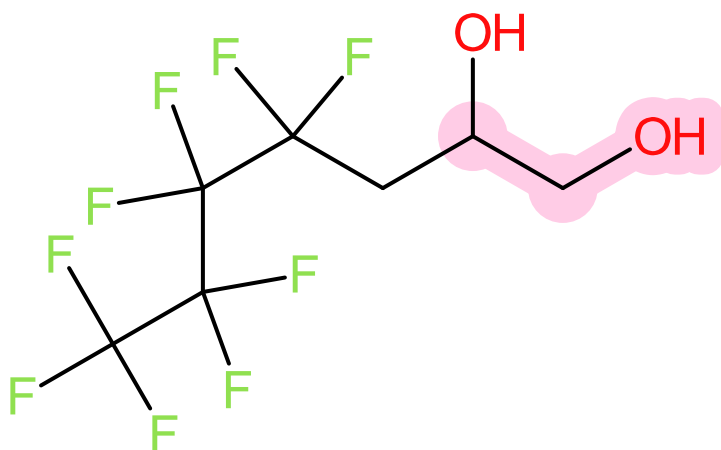
SGR10668 (2 chem)

SGR10703 (2 chem)

SGR10633

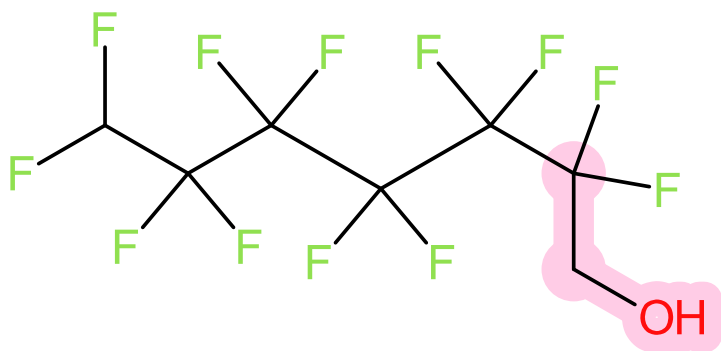
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



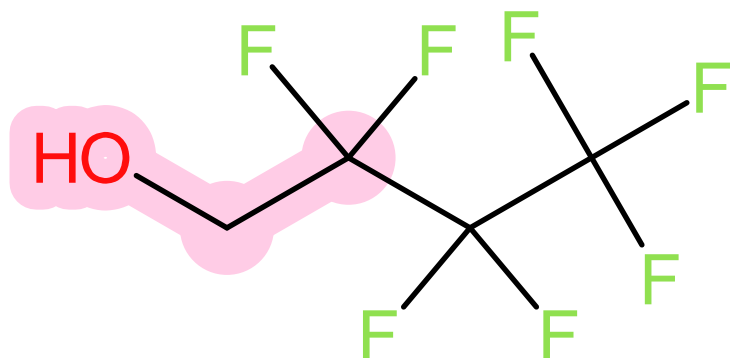
S7: Dodecafluoroheptanol (7H 6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F



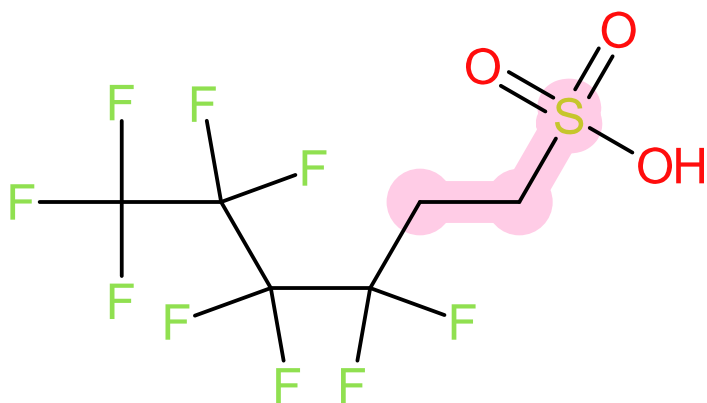
S12: Heptafluorobutanol (HpFBOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)F



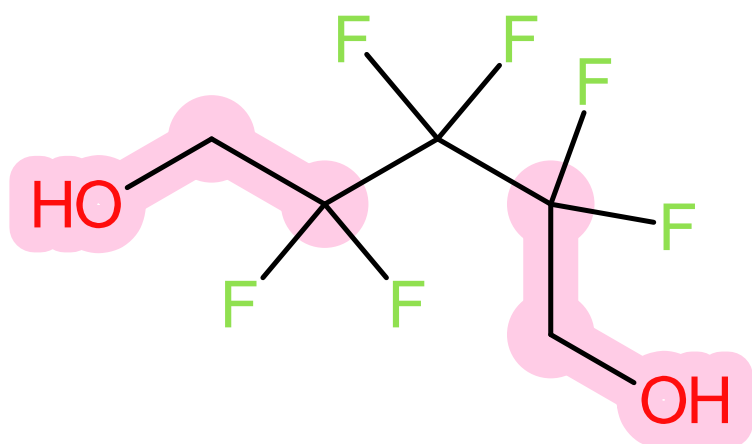
S13: 4:2 Fluorotelomer sulfonic acid (4:2 FTS)

SMILES: OS(=O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



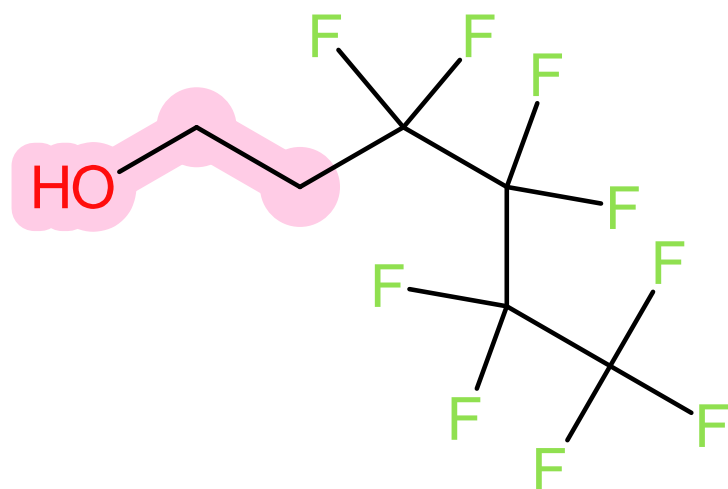
S14: Hexafluoroamylene glycol (CFH_x2OH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)CO



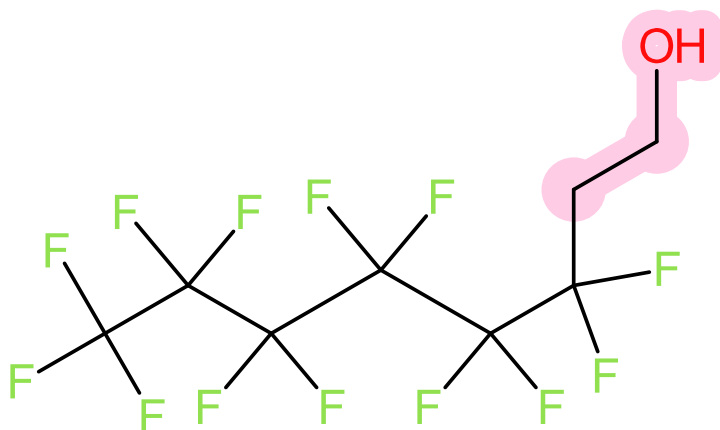
S21: 4:2 Fluorotelomer alcohol (4:2 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



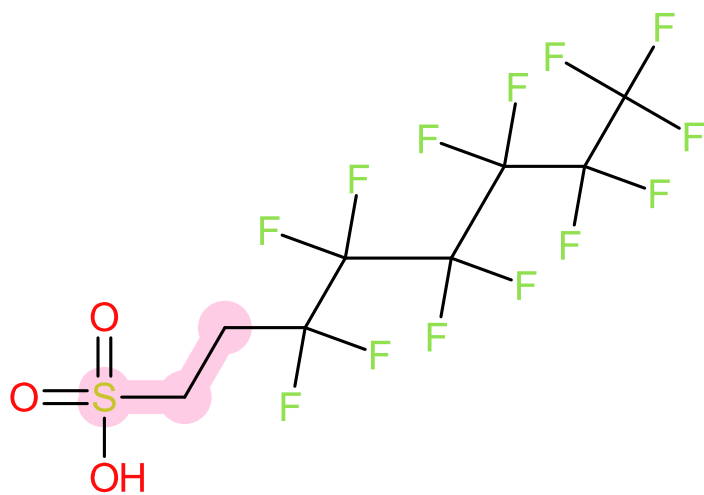
S26: 6:2 Fluorotelomer alcohol (6:2 FTOH)

SMILES: OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



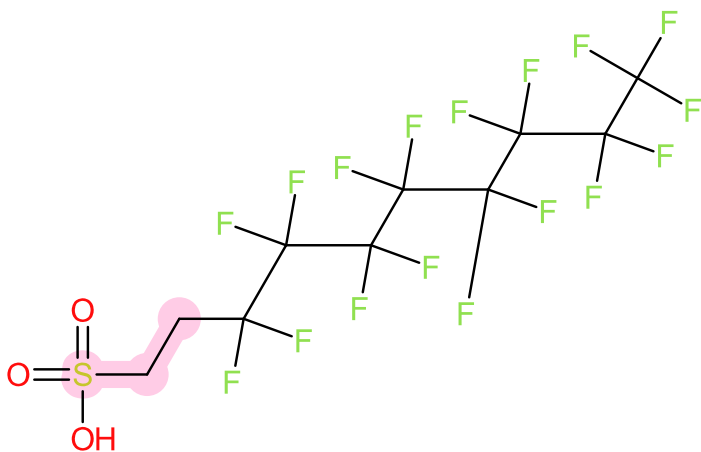
S32: 6:2 Fluorotelomer sulfonic acid (6:2 FTS)

SMILES: OS(=O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



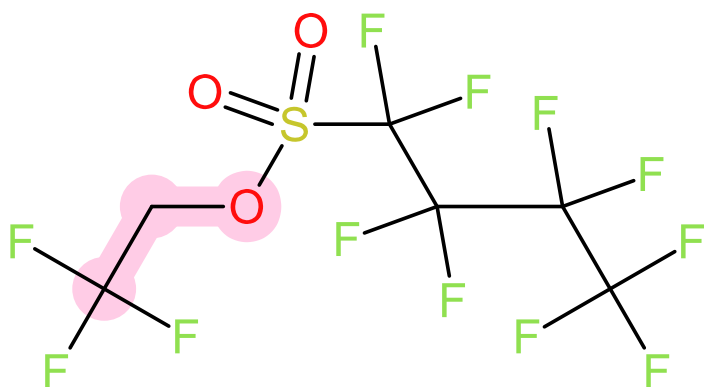
S33: 8:2 Fluorotelomer sulfonic acid (8:2 FTS)

SMILES: OS(=O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



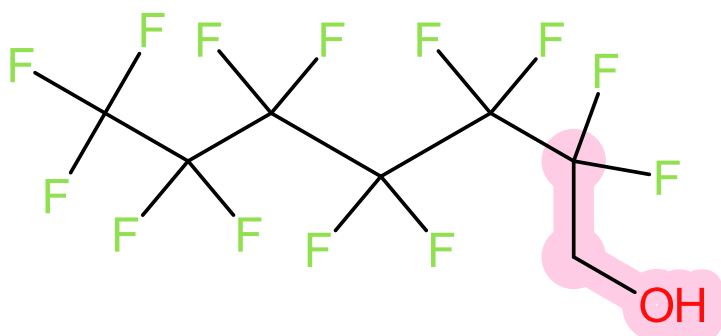
S38: 2,2,2-Trifluoroethyl perfluorobutanesulfonate (ET-PFBS)

SMILES: FC(F)(F)COS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



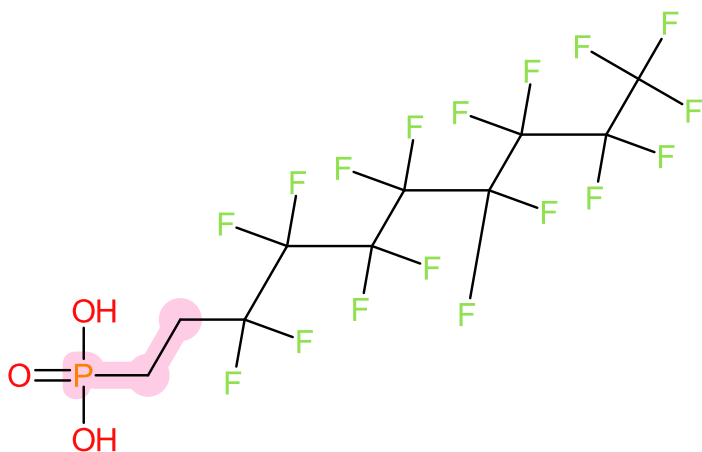
S47: 6:1 Fluorotelomer alcohol (6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



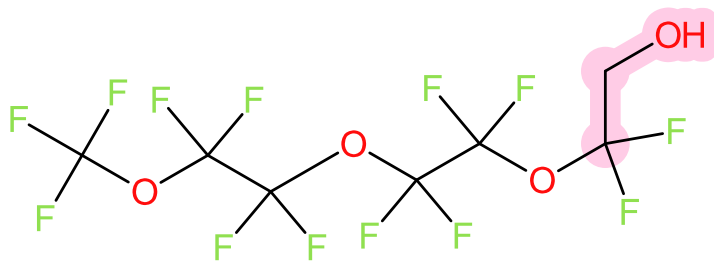
S52: ((Perfluorooctyl)ethyl)phosphonic acid (8:2 FTPA)

SMILES: OP(O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

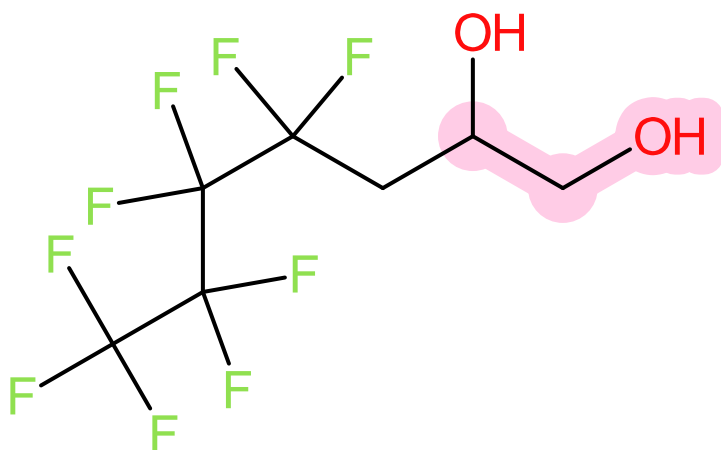
ID_56 OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10708

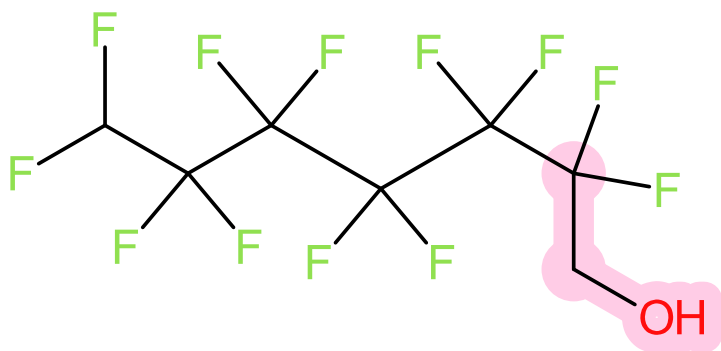
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F

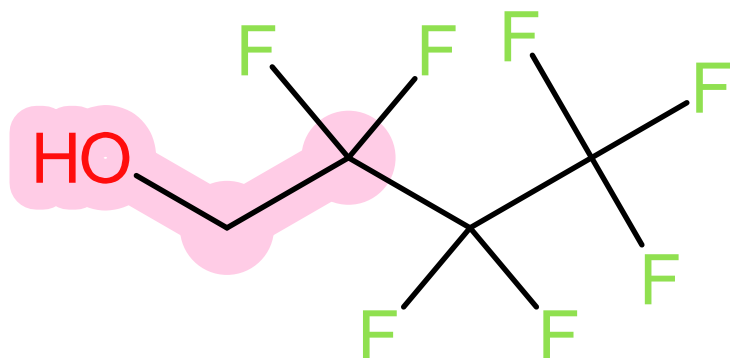


S7: Dodecafluoroheptanol (7H 6:1 FTOH)

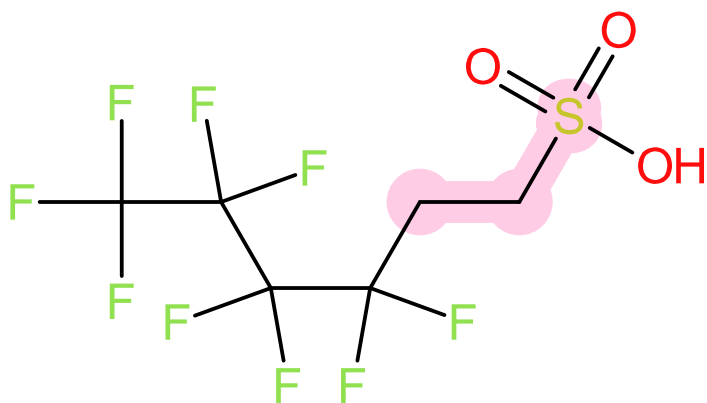
SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S12: Heptafluorobutanol (HpFBOH)
SMILES: OCC(F)(F)C(F)(F)C(F)(F)F

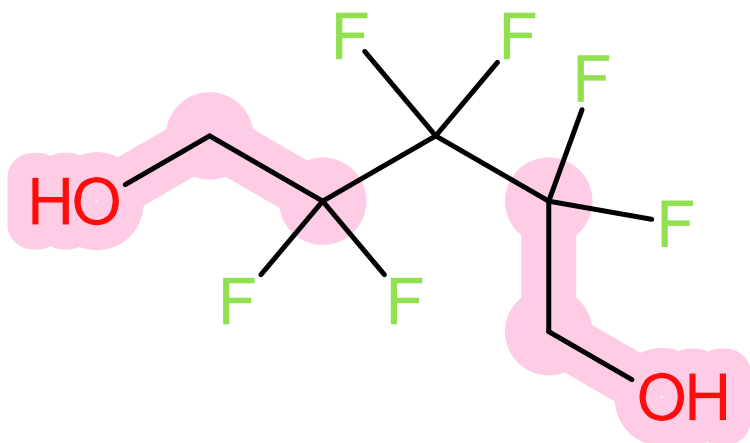


S13: 4:2 Fluorotelomer sulfonic acid (4:2 FTS)
SMILES: OS(=O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



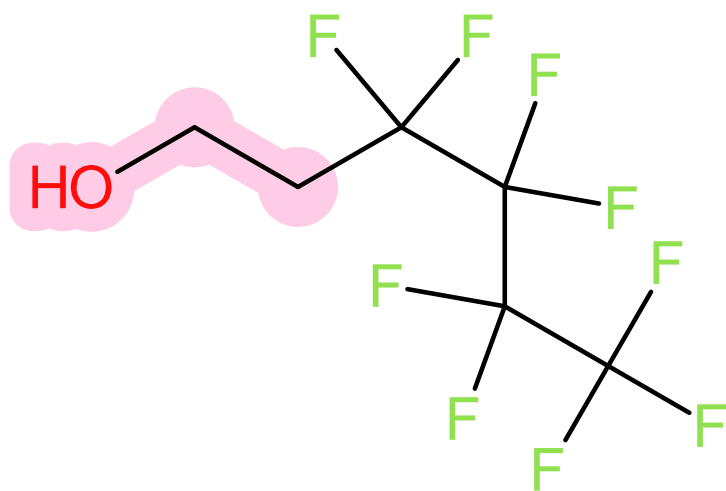
S14: Hexafluoroamylene glycol (CFH_x2OH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)CO

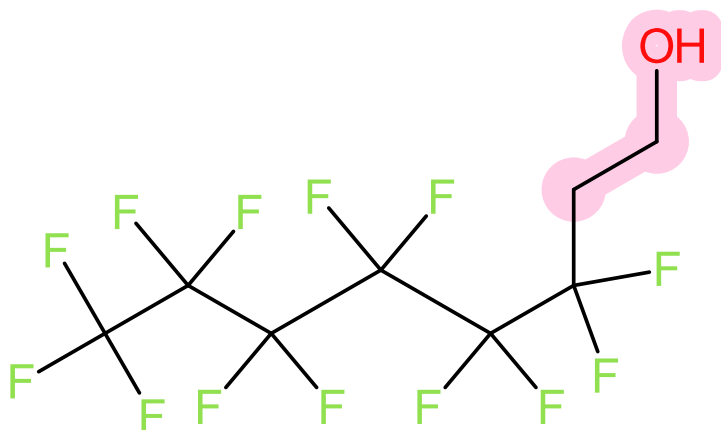


S21: 4:2 Fluorotelomer alcohol (4:2 FTOH)

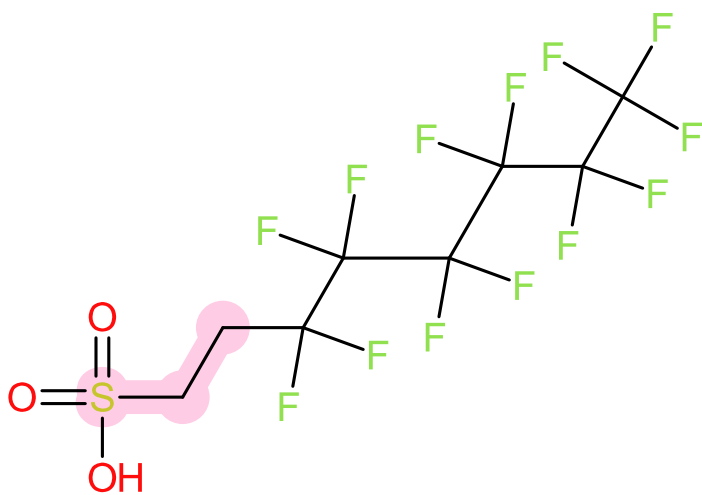
SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S26: 6:2 Fluorotelomer alcohol (6:2 FTOH)
ID_26 OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

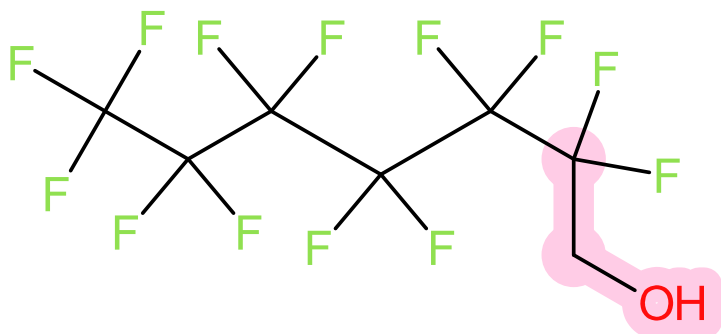


S32: 6:2 Fluorotelomer sulfonic acid (6:2 FTS)
SMILES: OS(=O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



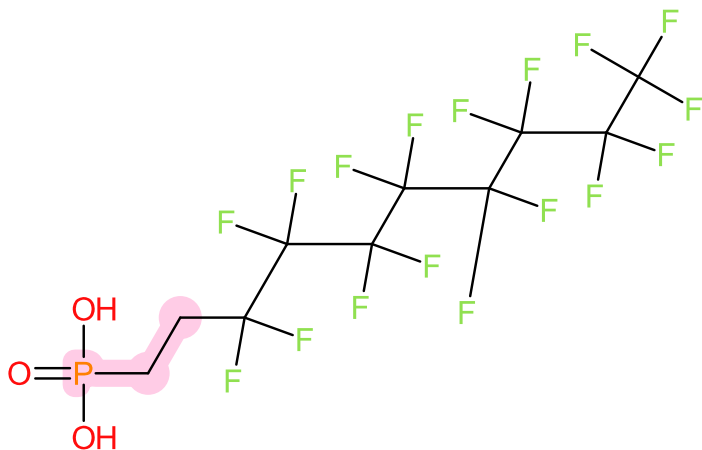
S47: 6:1 Fluorotelomer alcohol (6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



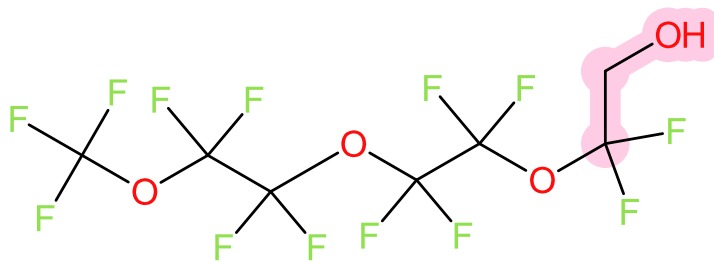
S52: ((Perfluorooctyl)ethyl)phosphonic acid (8:2 FTPA)

SMILES: OP(O)(=O)CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

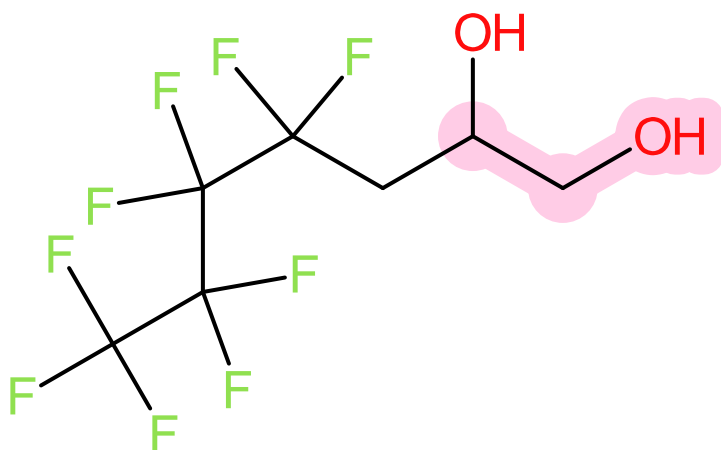
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10275

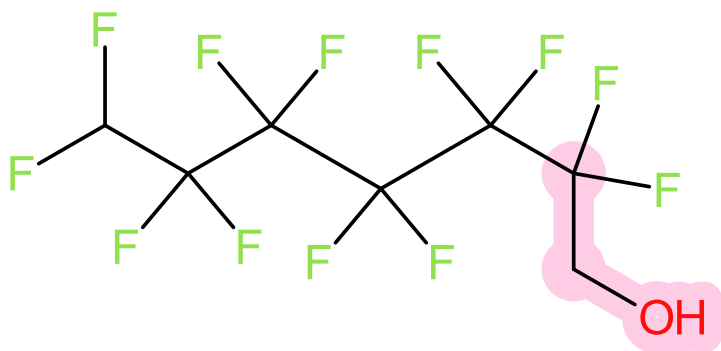
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F

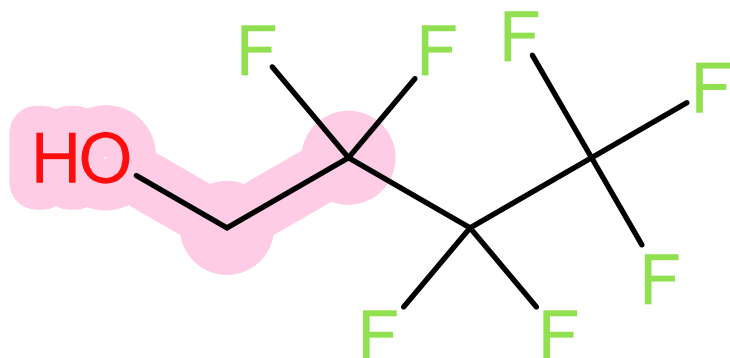


S7: Dodecafluoroheptanol (7H 6:1 FTOH)

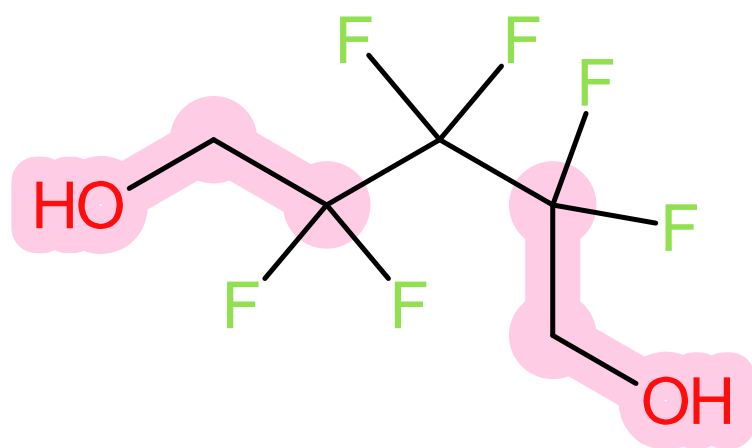
SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



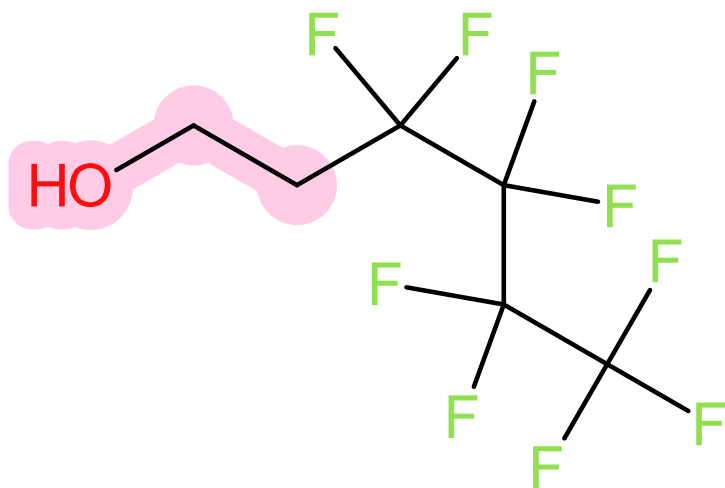
S12: Heptafluorobutanol (HpFBOH)
SMILES: OCC(F)(F)C(F)(F)C(F)(F)F



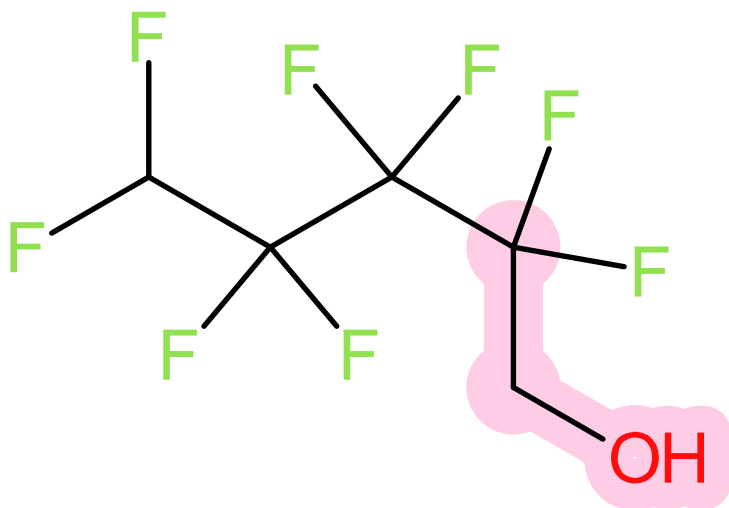
S14: Hexafluoroamylene glycol (CFHx2OH)
SMILES: OCC(F)(F)C(F)(F)C(F)(F)CO



S21: 4:2 Fluorotelomer alcohol (4:2 FTOH)
SMILES: OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F

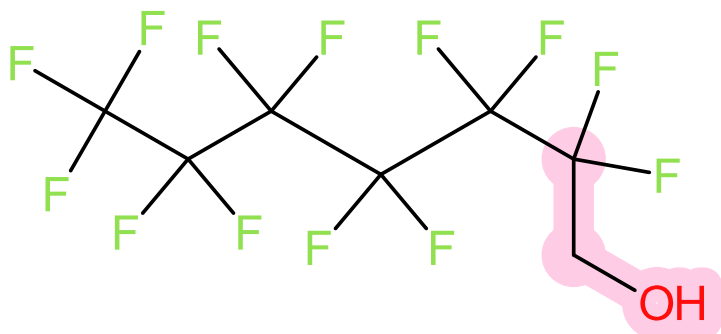


S23: 1H,1H,5H-Perfluoropentanol (PFPOH)
SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)F



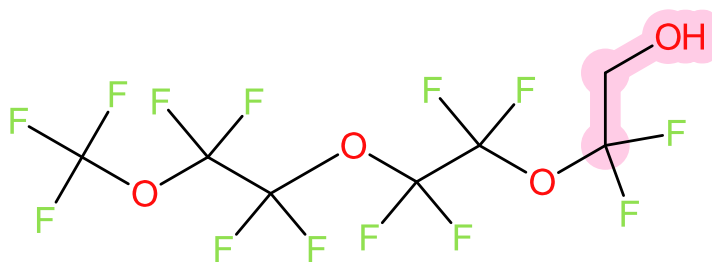
S47: 6:1 Fluorotelomer alcohol (6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

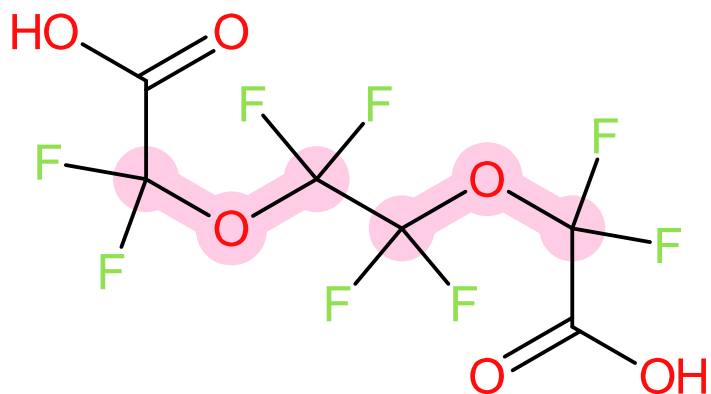
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10169

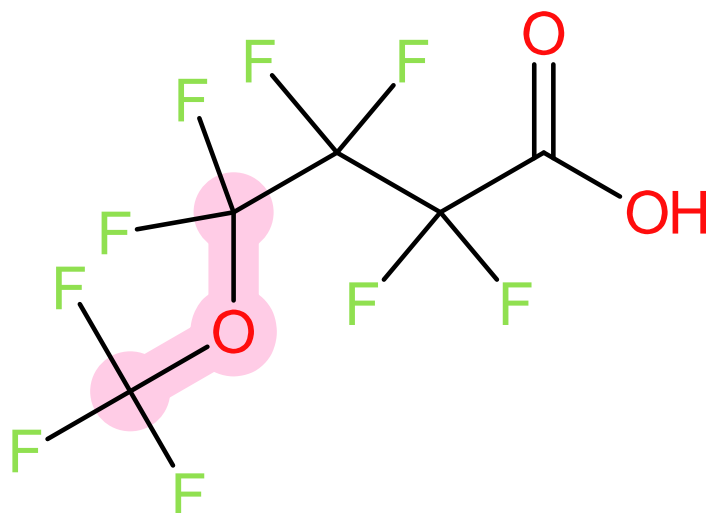
S3: Perfluoro-3,6-dioxaoctane-1,8-dioic acid (PFHx2Et2OA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(O)=O



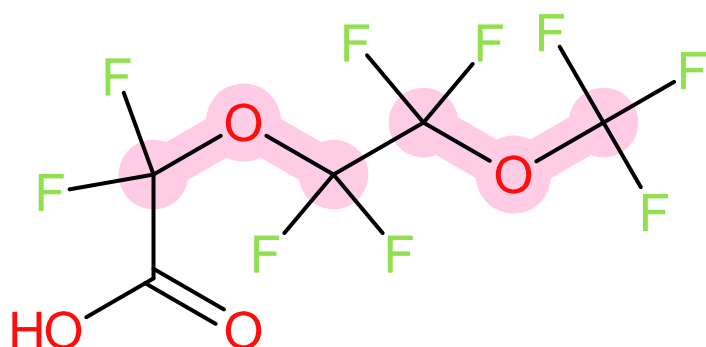
S9: Perfluoro(4-methoxybutanoic) acid (PFMBA)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)F



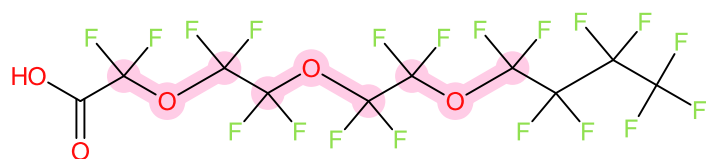
S11: Perfluoro-3,6-dioxaheptanoic acid (NFDHA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



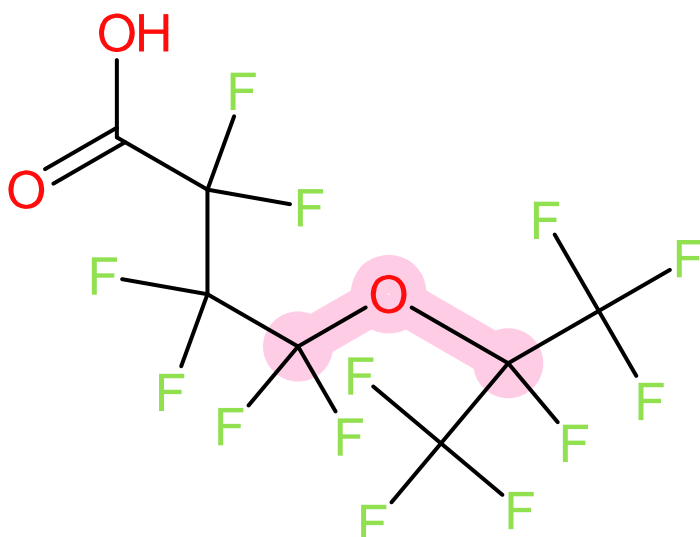
S22: Perfluoro-3,6,9-trioxatridecanoic acid (PFPE-6)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



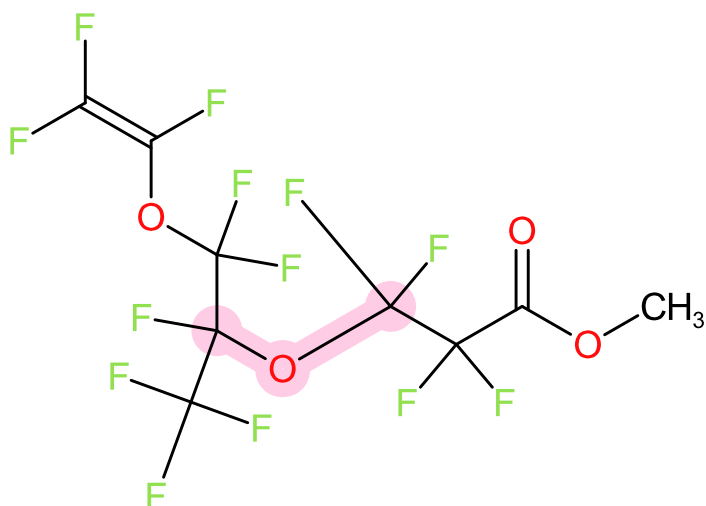
S36: Perfluoro-4-isopropoxybutanoic acid (PFPE-1)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)F



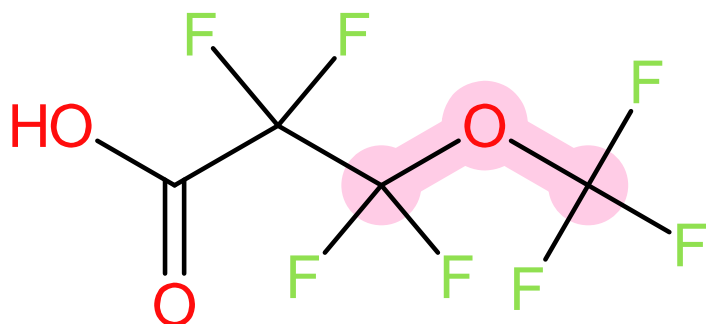
S39: Methyl perfluoro(3-(1-ethenyloxypropan-2-yloxy)propanoate) (MePF2ETOA)

SMILES: COC(=O)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)=C(F)F



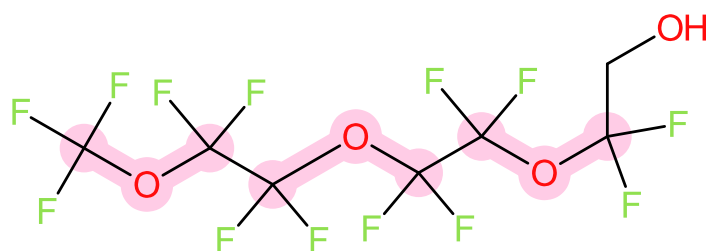
S49: Perfluoro-3-methoxypropanoic acid (PFMPA)

SMILES: OC(=O)C(F)(F)C(F)(F)OC(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C₇F₃ETOH)

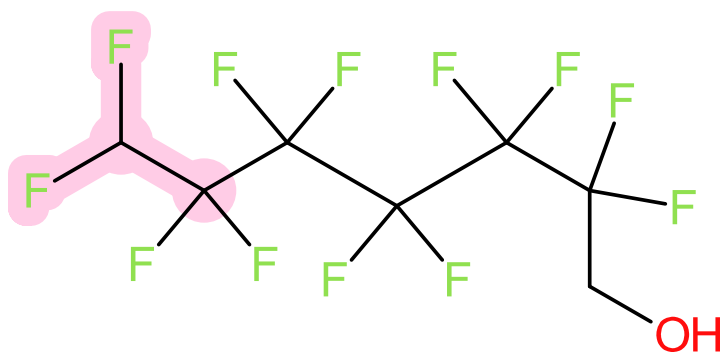
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10795

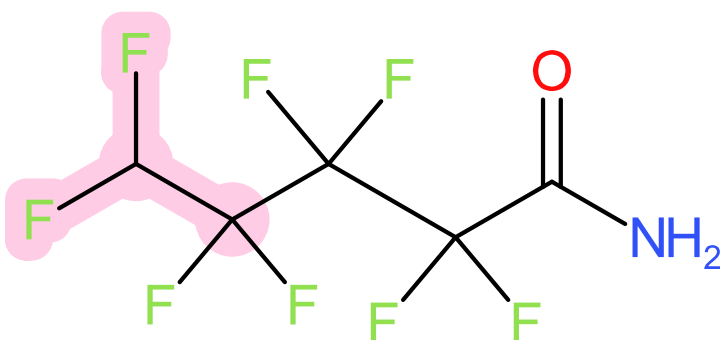
S7: Dodecafluoroheptanol (7H 6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F



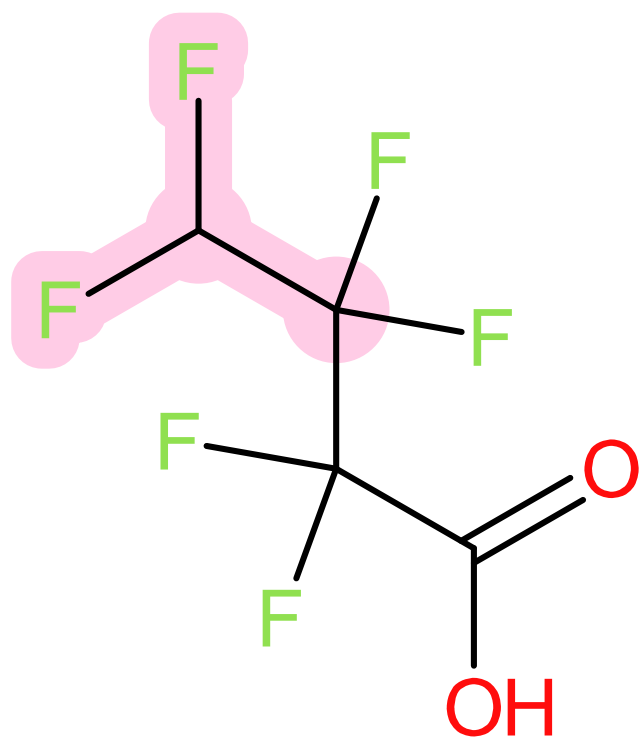
S16: Perfluoropentanamide (PFPAM)

SMILES: NC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)F



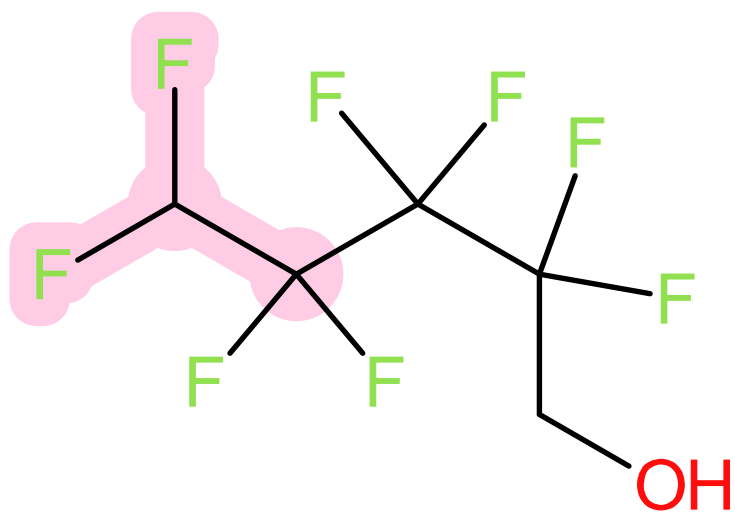
S17: 2,2,3,3,4,4-Hexafluorobutanoic acid (4H-PFBA)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)F



S23: 1H,1H,5H-Perfluoropentanol (PFPOH)

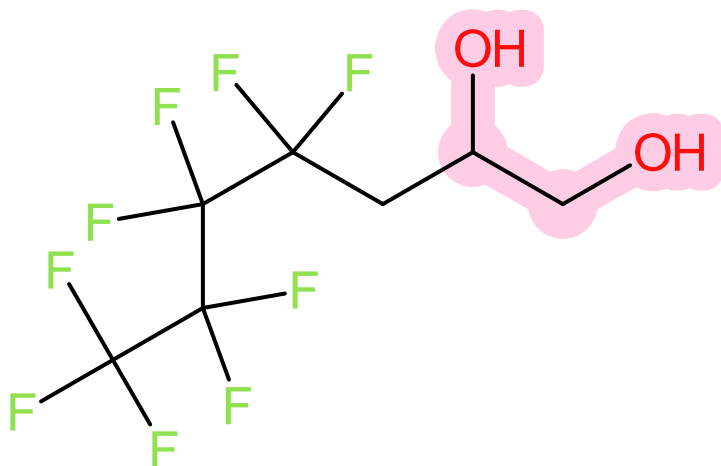
SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)F



SGR10290

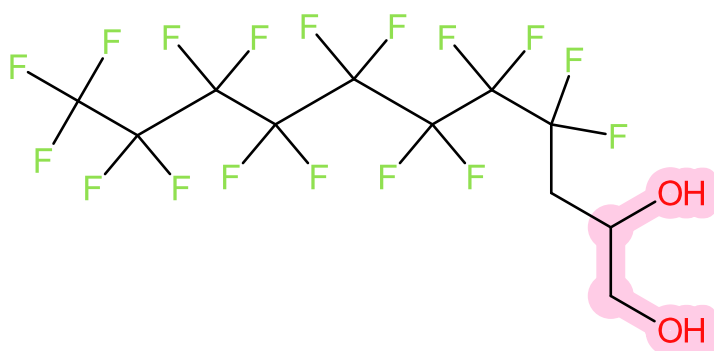
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



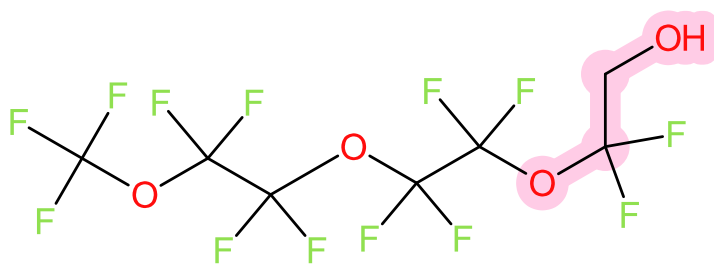
S40: 1-(Perfluorooctyl)propane-2,3-diol (PFUd2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

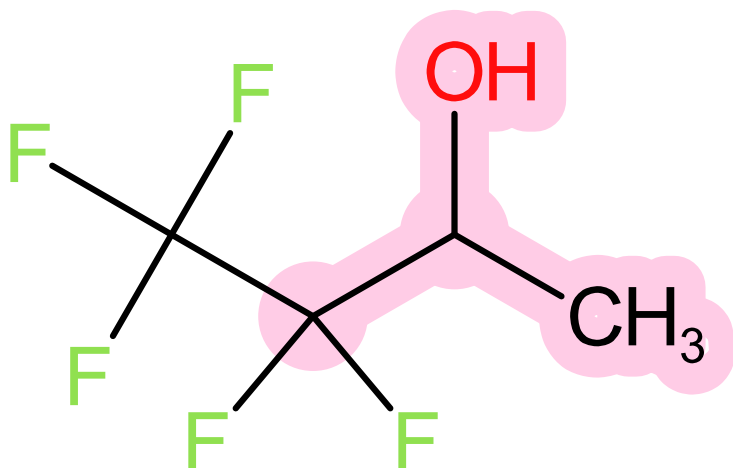
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10418

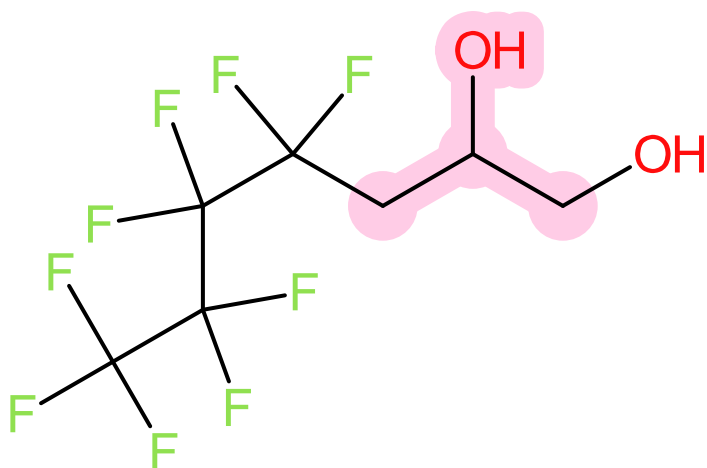
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

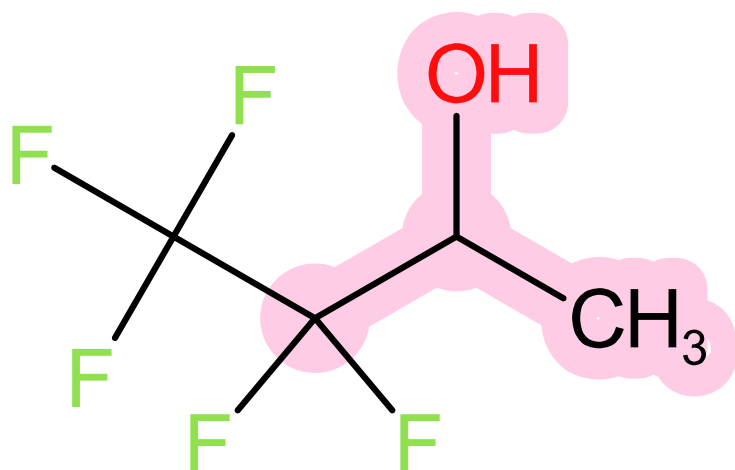
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10493

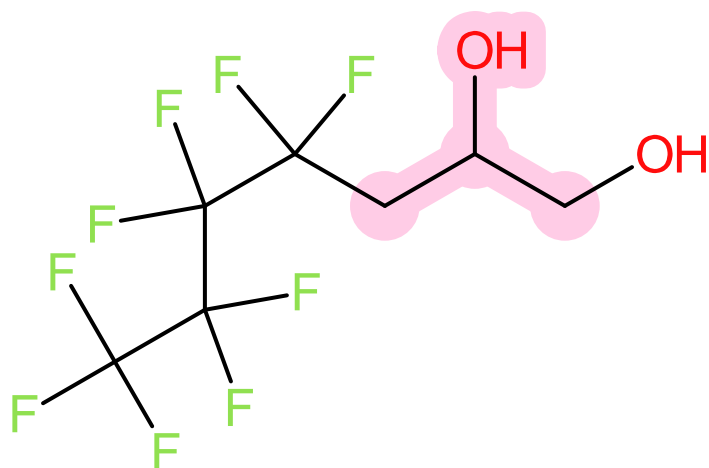
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

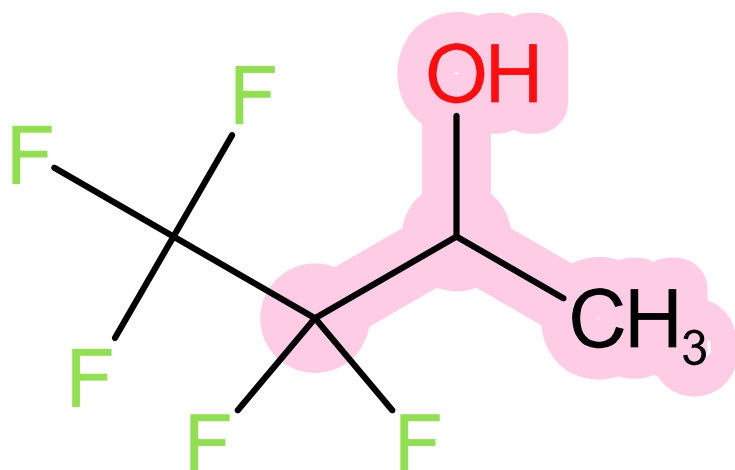
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10684

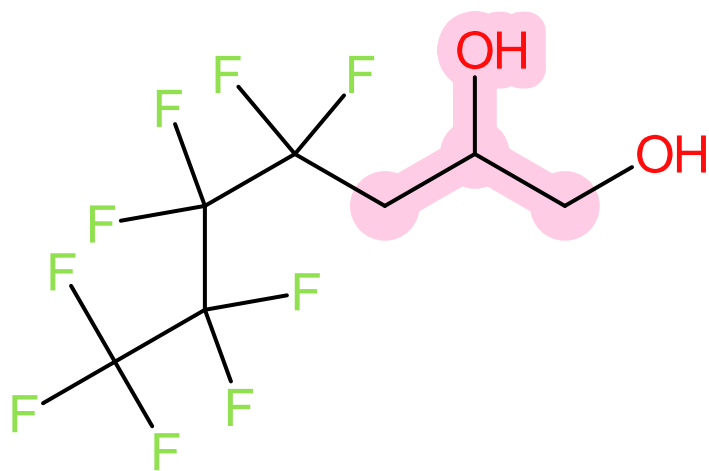
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

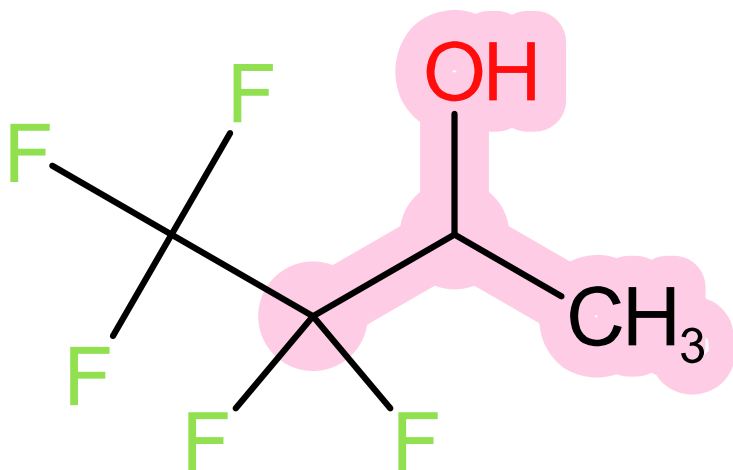
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10736

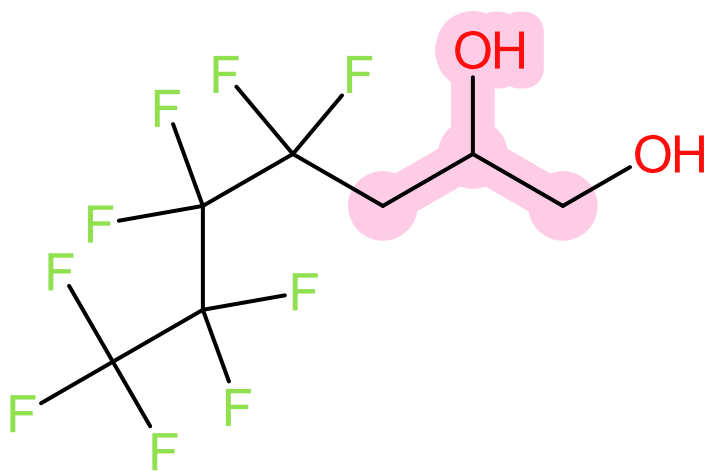
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

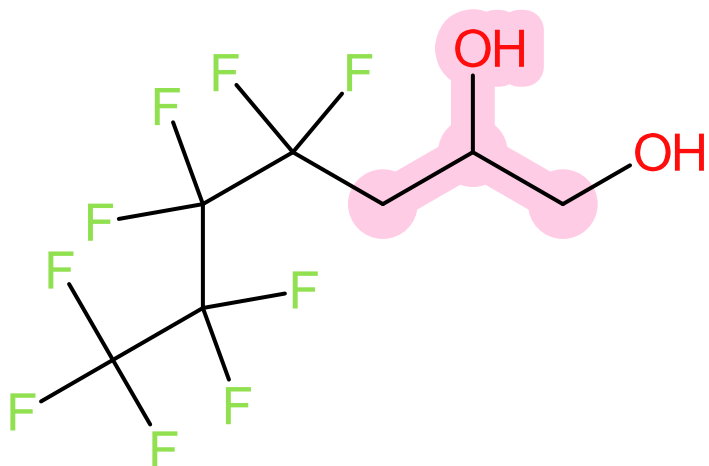
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10354

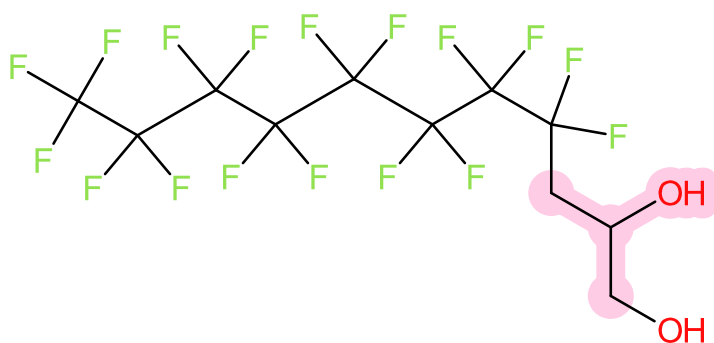
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S40: 1-(Perfluorooctyl)propane-2,3-diol (PFUd2OH)

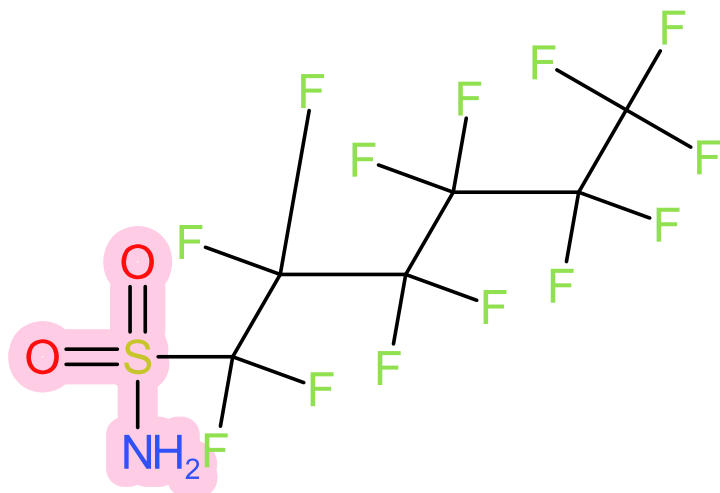
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10703

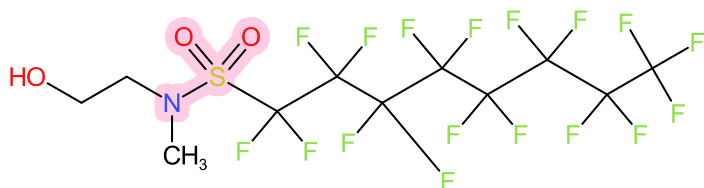
S31: Perfluorohexanesulfonamide (PFHxSA)

SMILES: NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S43: N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide (MeFOSE)

SMILES: CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



FUNCTIONAL GROUPS

SGR10072 (14 chem)

SGR10761 (14 chem)

SGR10295 (12 chem)

SGR10203 (8 chem)

SGR10153 (7 chem)

SGR10109 (3 chem)

SGR10343 (3 chem)

SGR10099 (2 chem)

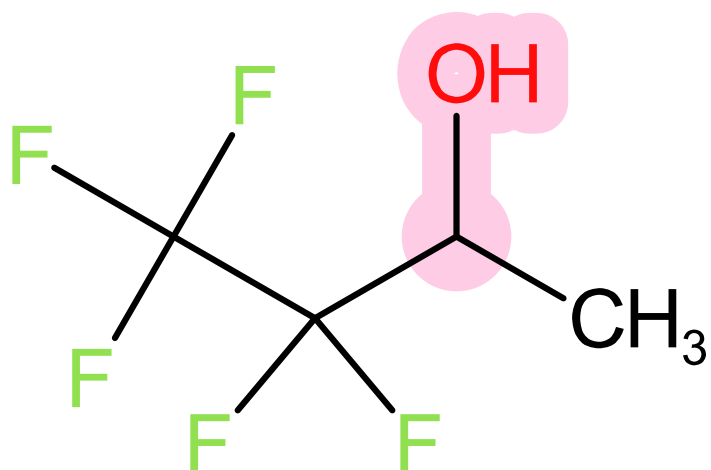
SGR10289 (2 chem)

SGR10587 (2 chem)

SGR10072

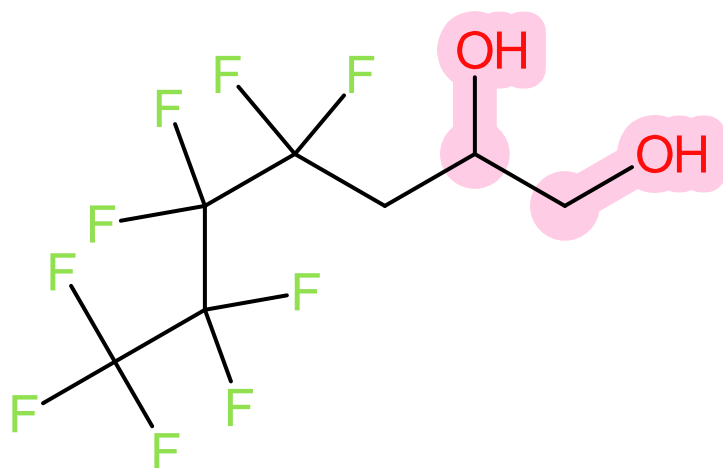
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



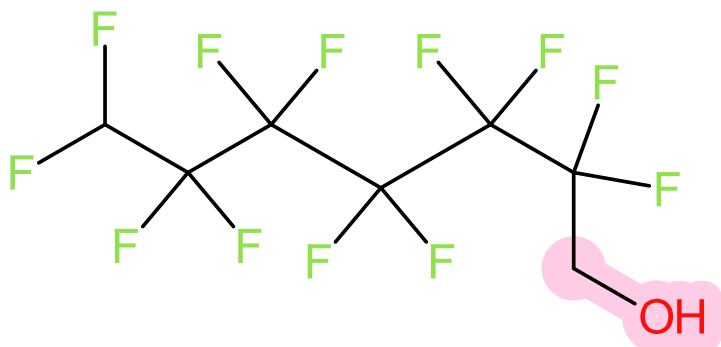
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



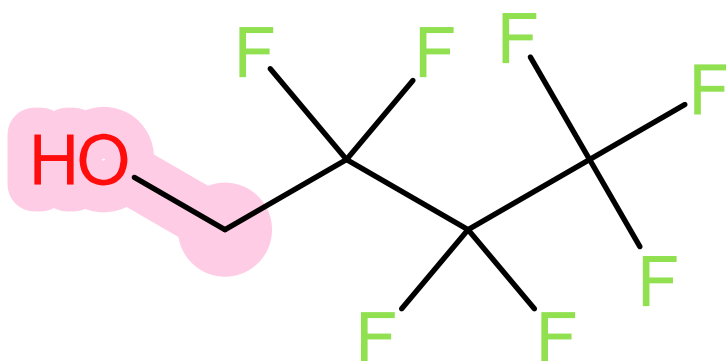
S7: Dodecafluoroheptanol (7H 6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F



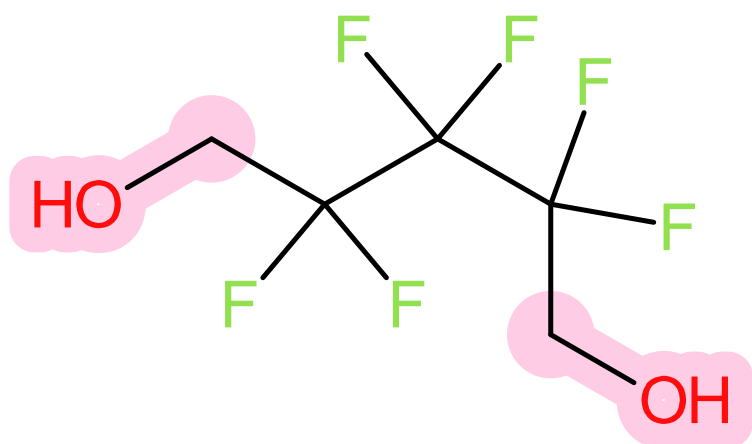
S12: Heptafluorobutanol (HpFBOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)F



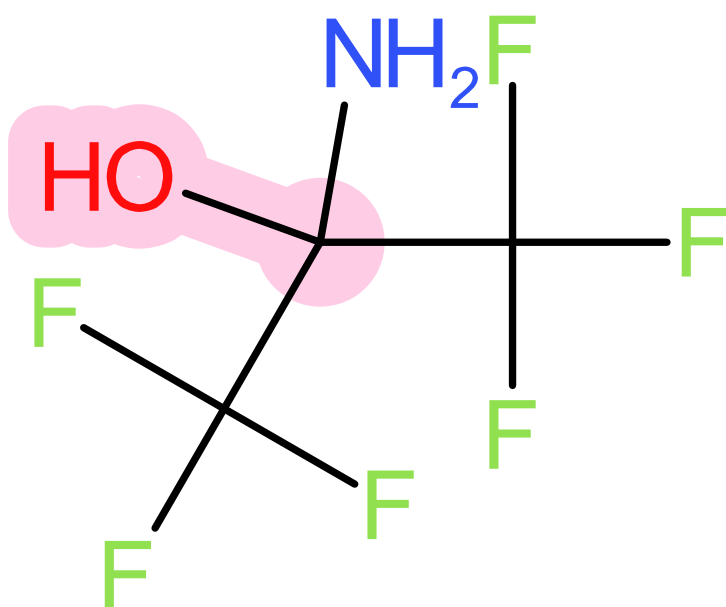
S14: Hexafluoroamylene glycol (CFH_x2OH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)CO



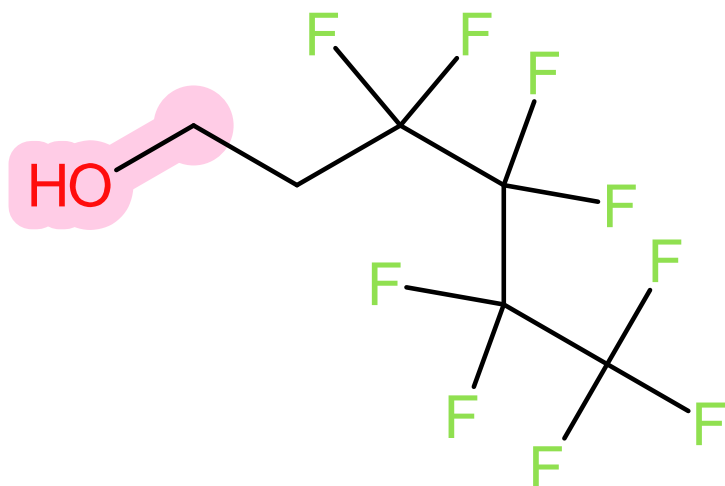
S20: 2-Aminohexafluoropropan-2-ol (AmFPrOH)

SMILES: NC(O)(C(F)(F)F)C(F)(F)F



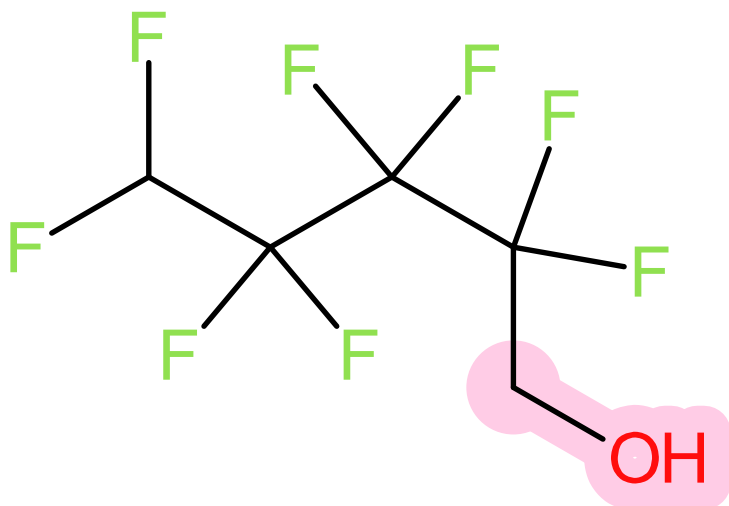
S21: 4:2 Fluorotelomer alcohol (4:2 FTOH)

SMILES: OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



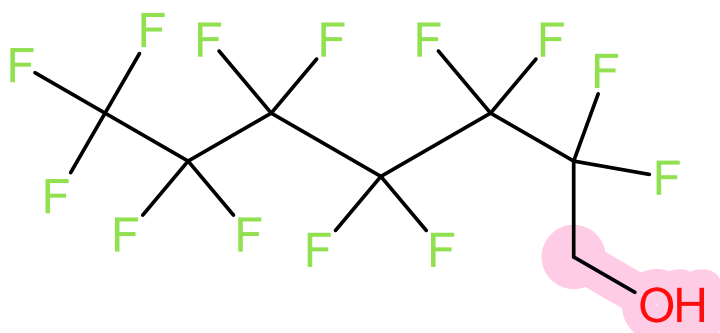
S23: 1H,1H,5H-Perfluoropentanol (PFPOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)F



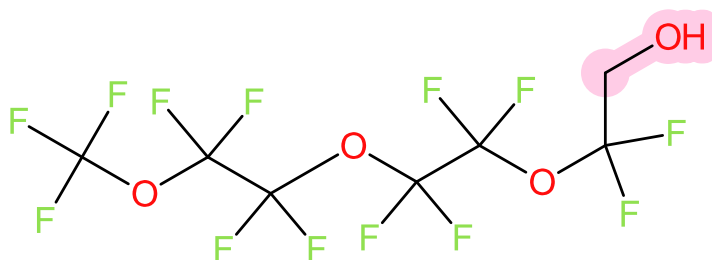
S47: 6:1 Fluorotelomer alcohol (6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

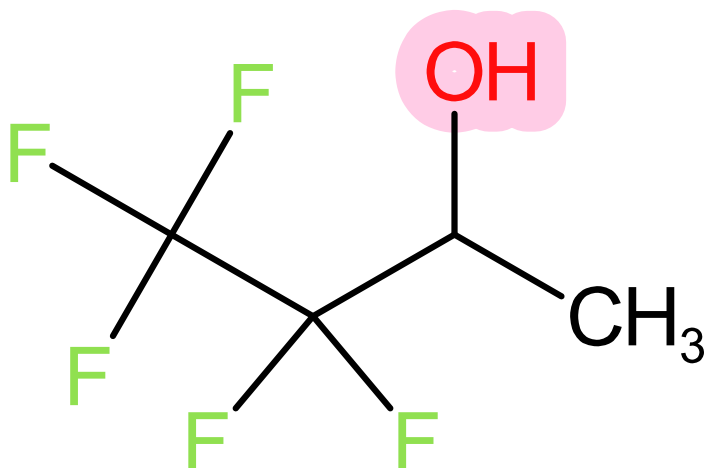
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10761

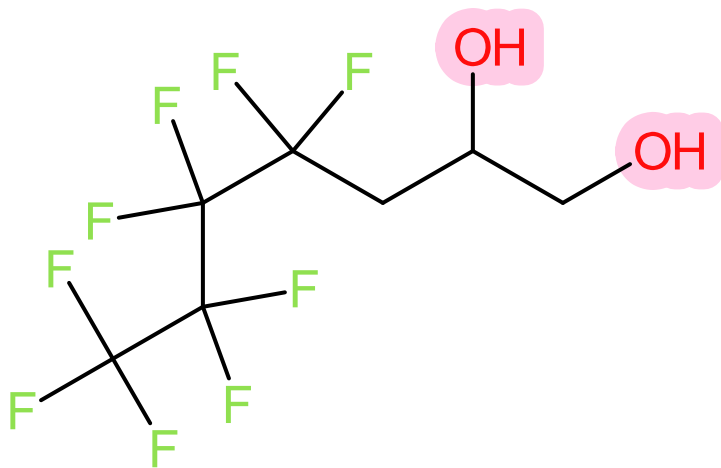
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



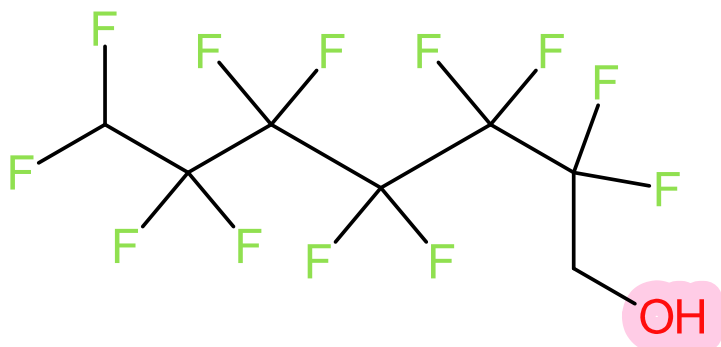
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



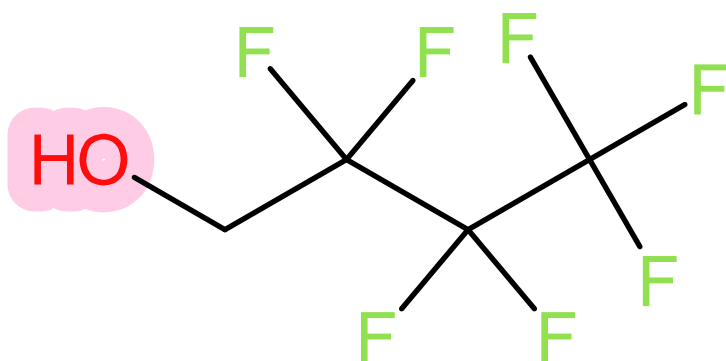
S7: Dodecafluoroheptanol (7H 6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F



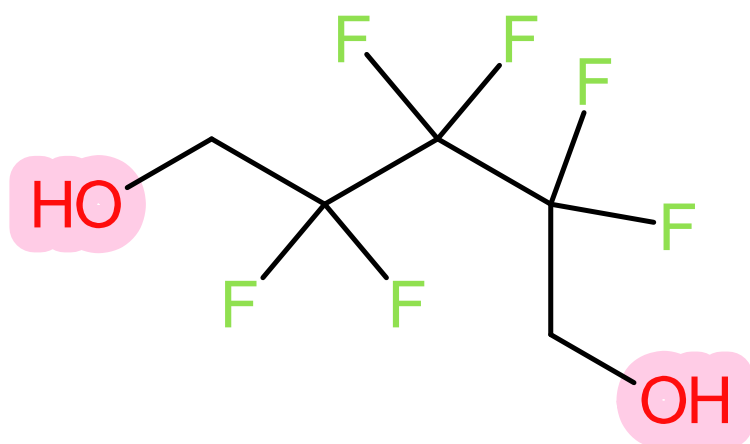
S12: Heptafluorobutanol (HpFBOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)F



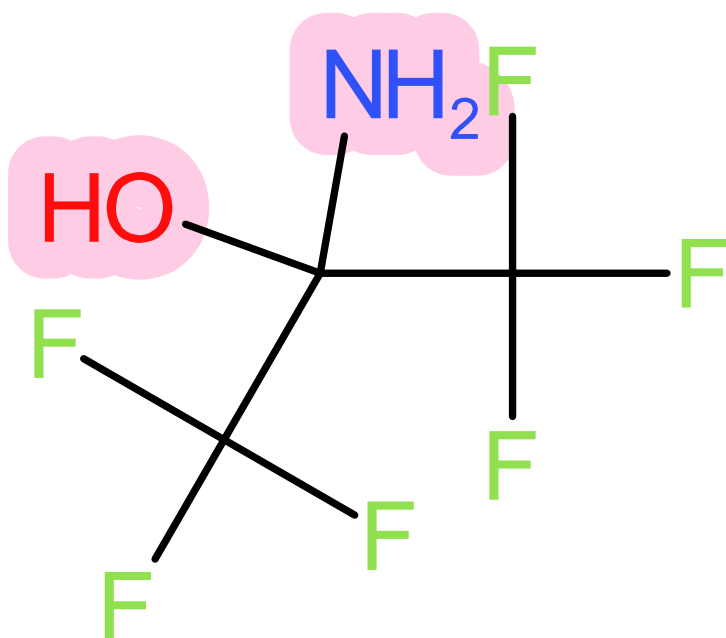
S14: Hexafluoroamylene glycol (CFH_x2OH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)CO

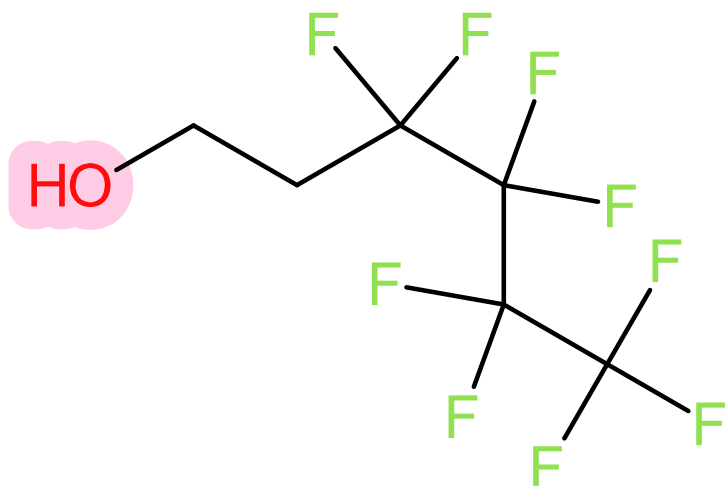


S20: 2-Aminohexafluoropropan-2-ol (AmFPrOH)

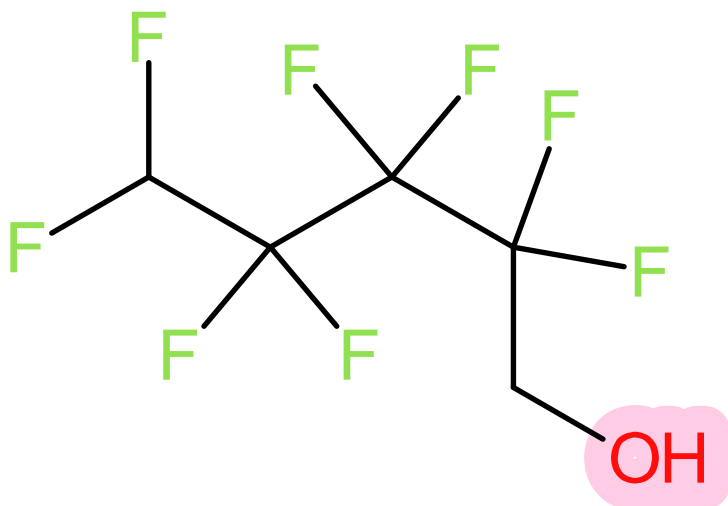
SMILES: NC(O)(C(F)(F)F)C(F)(F)F



S21: 4:2 Fluorotelomer alcohol (4:2 FTOH)
SMILES: OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F

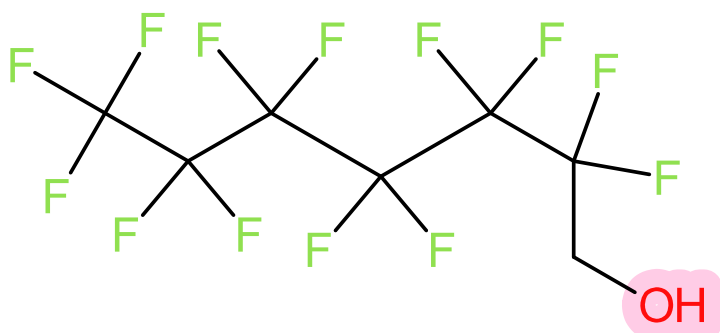


S23: 1H,1H,5H-Perfluoropentanol (PFPOH)
SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)F



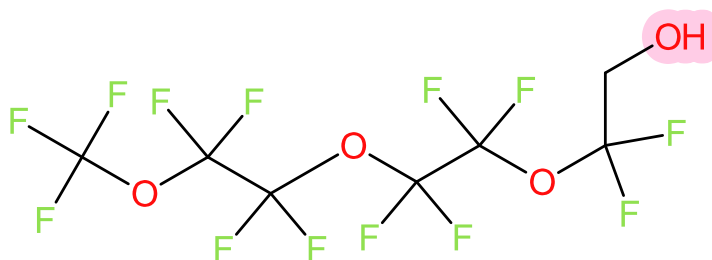
S47: 6:1 Fluorotelomer alcohol (6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

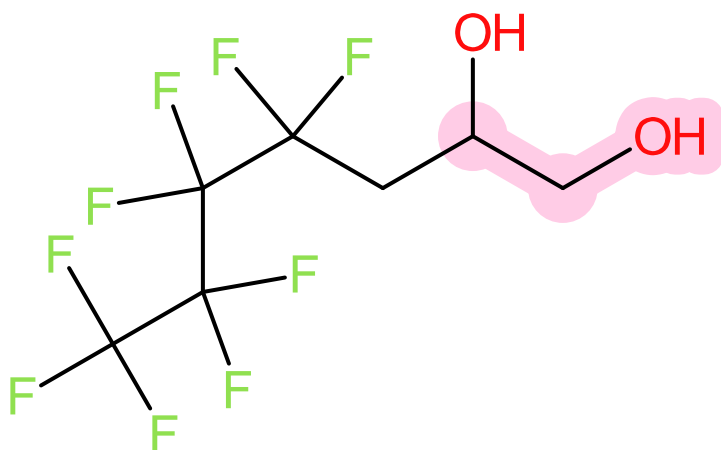
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10295

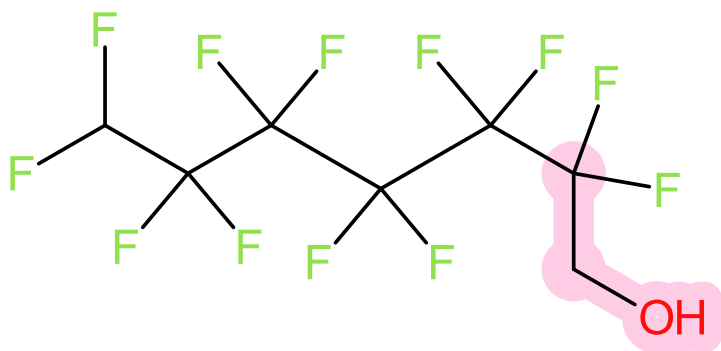
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



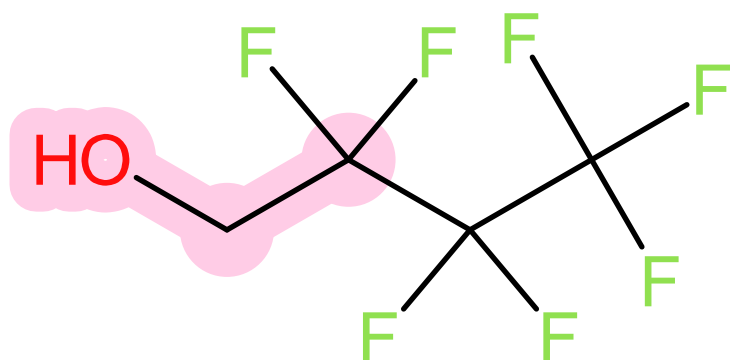
S7: Dodecafluoroheptanol (7H 6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



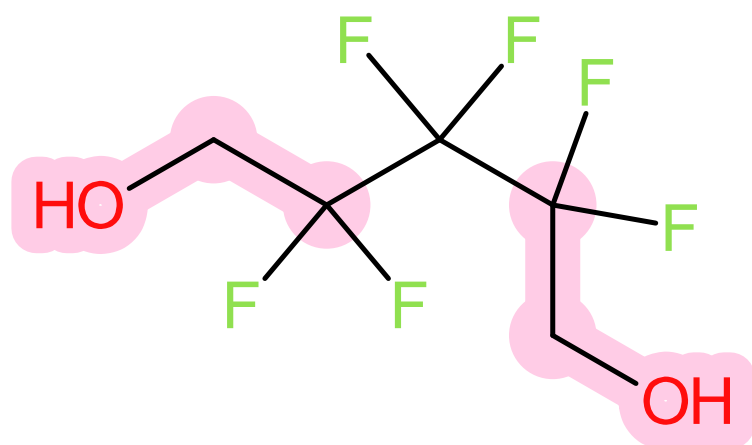
S12: Heptafluorobutanol (HpFBOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)F



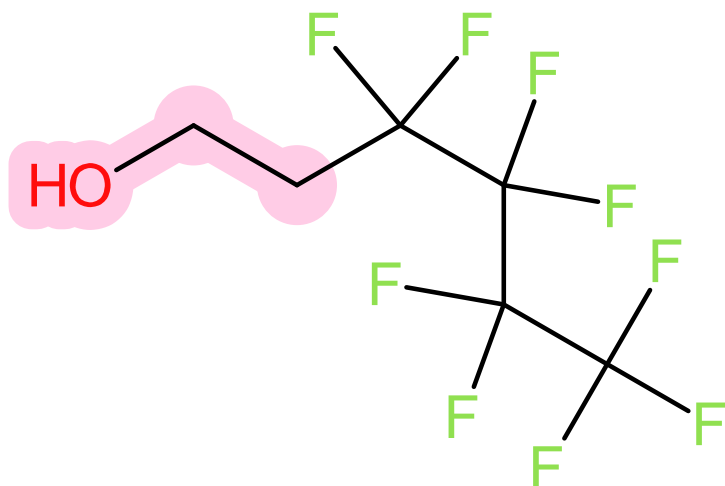
S14: Hexafluoroamylene glycol (CFH₂O₂H)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)CO



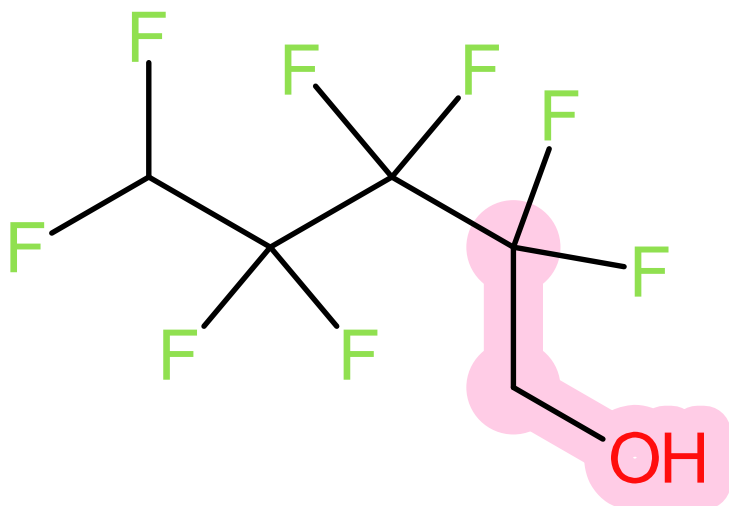
S21: 4:2 Fluorotelomer alcohol (4:2 FTOH)

SMILES: OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



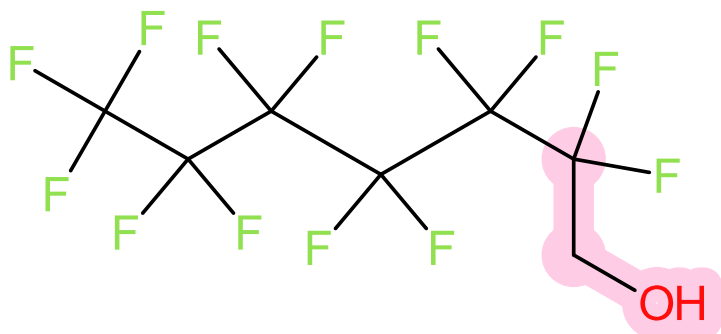
S23: 1H,1H,5H-Perfluoropentanol (PFPOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)F



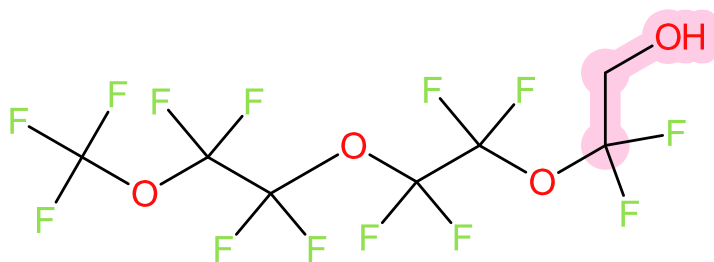
S47: 6:1 Fluorotelomer alcohol (6:1 FTOH)

SMILES: OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

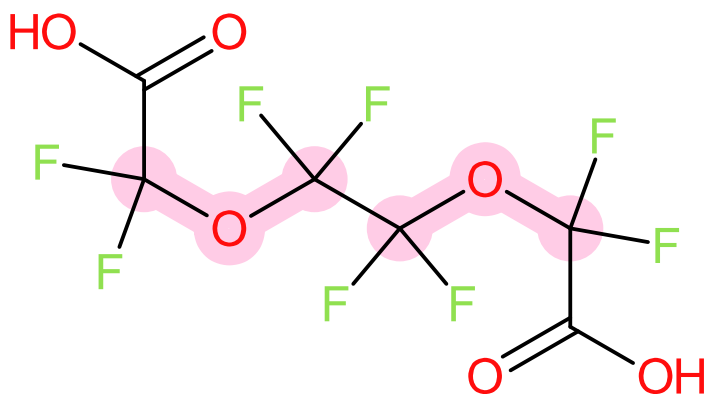
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10203

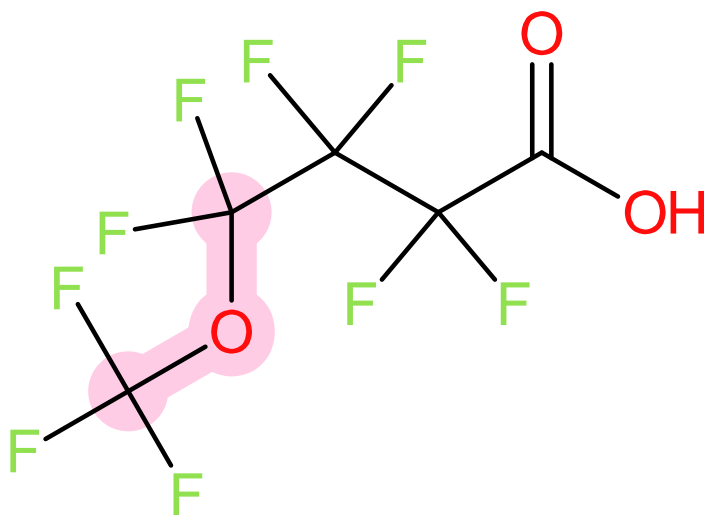
S3: Perfluoro-3,6-dioxaoctane-1,8-dioic acid (PFHx2Et2OA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(O)=O



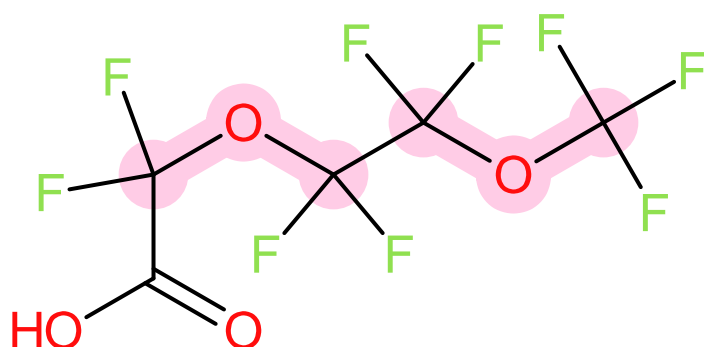
S9: Perfluoro(4-methoxybutanoic) acid (PFMBA)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)F



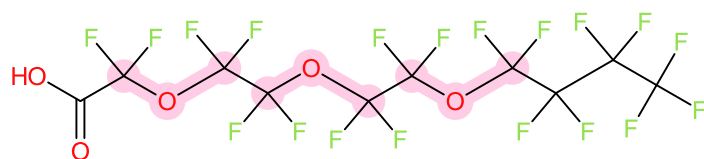
S11: Perfluoro-3,6-dioxaheptanoic acid (NFDHA)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



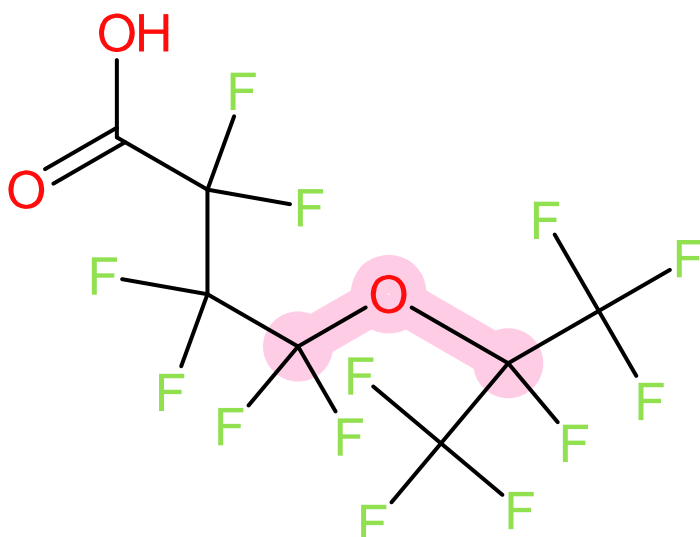
S22: Perfluoro-3,6,9-trioxatridecanoic acid (PFPE-6)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



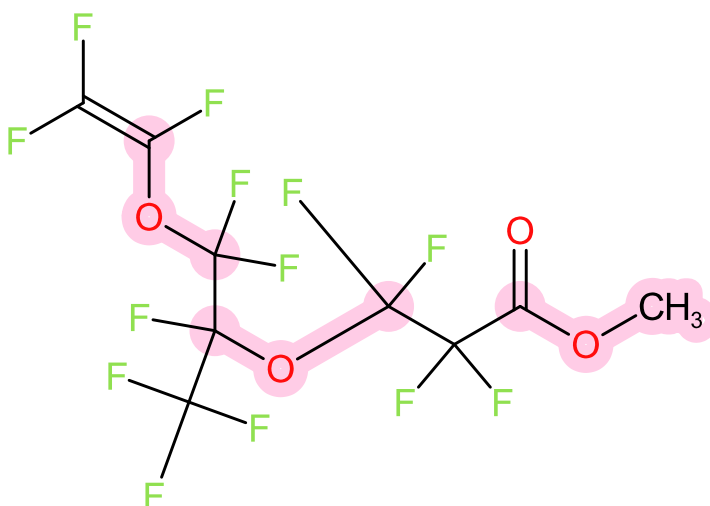
S36: Perfluoro-4-isopropoxybutanoic acid (PFPE-1)

SMILES: OC(=O)C(F)(F)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)F



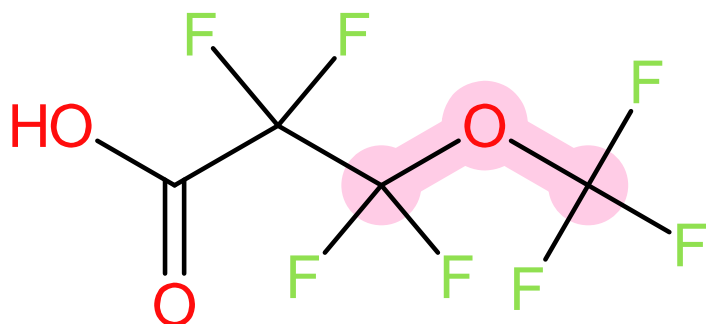
S39: Methyl perfluoro(3-(1-ethenyloxypropan-2-yloxy)propanoate) (MePF2ETOA)

SMILES: COC(=O)C(F)(F)C(F)(F)OC(F)(C(F)(F)F)C(F)(F)OC(F)=C(F)F



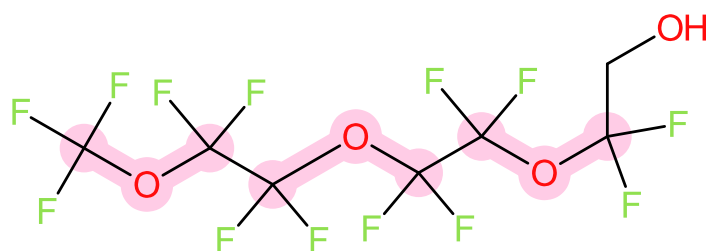
S49: Perfluoro-3-methoxypropanoic acid (PFMPA)

SMILES: OC(=O)C(F)(F)C(F)(F)OC(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

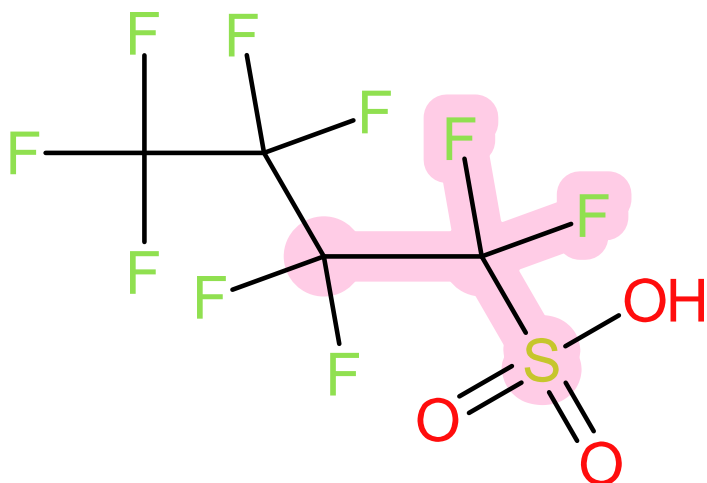
ID_56 OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10153

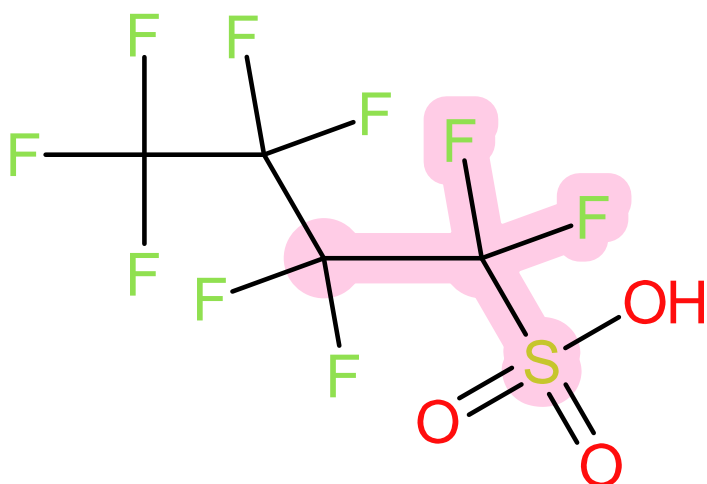
S10: Perfluorobutanesulfonic acid (PFBS)

SMILES: OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



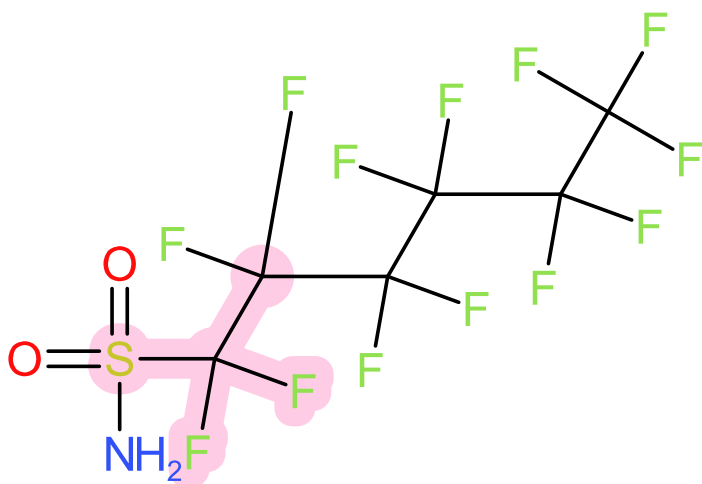
S29: Potassium perfluorobutanesulfonate (PFBS-K)

SMILES: OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



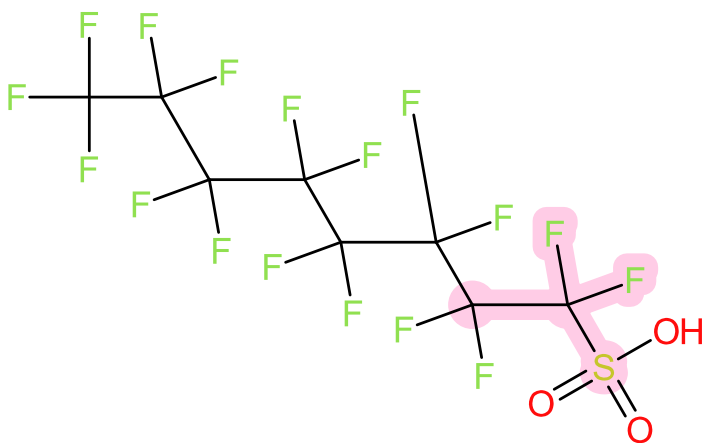
S31: Perfluorohexanesulfonamide (PFHxSA)

SMILES: NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



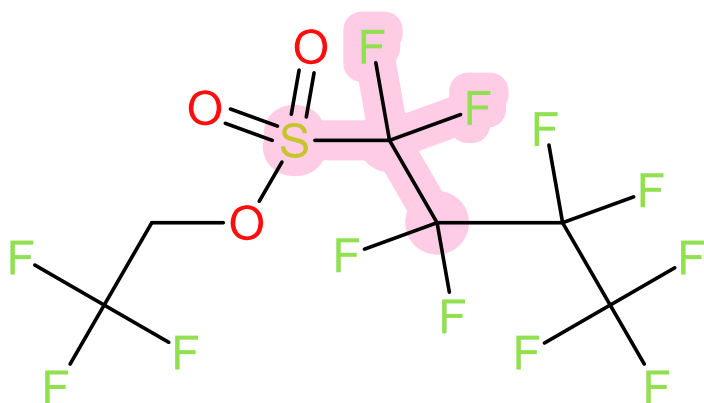
S37: Perfluorooctanesulfonic acid (PFOS)

SMILES: OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



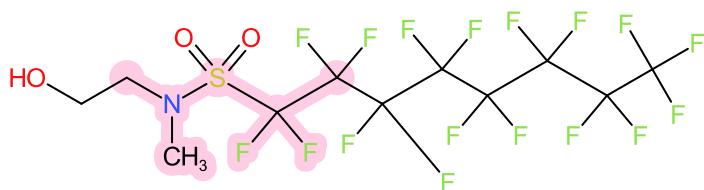
S38: 2,2,2-Trifluoroethyl perfluorobutanesulfonate (ET-PFBS)

SMILES: FC(F)(F)COS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



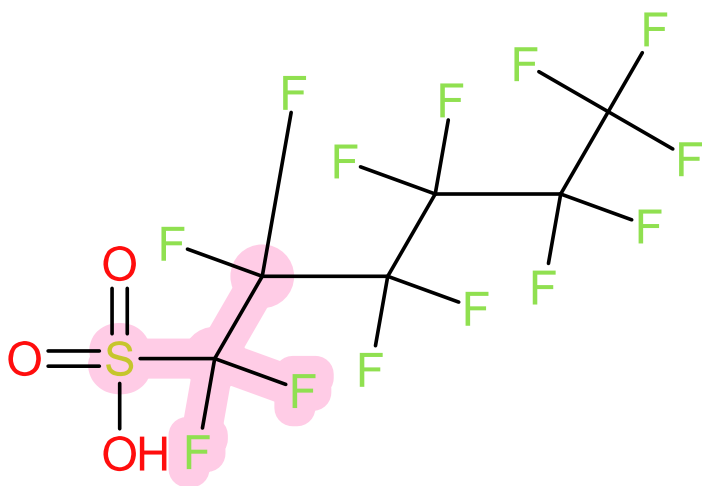
S43: N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide (MeFOSE)

SMILES: CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S51: Perfluorohexanesulfonic acid (PFHxS)

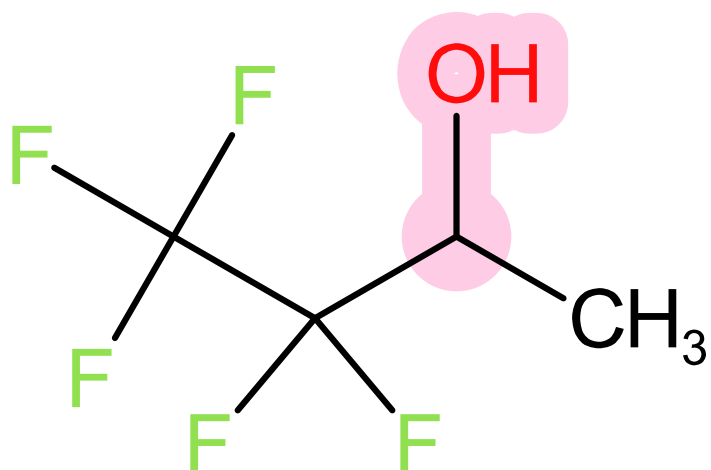
SMILES: OS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10109

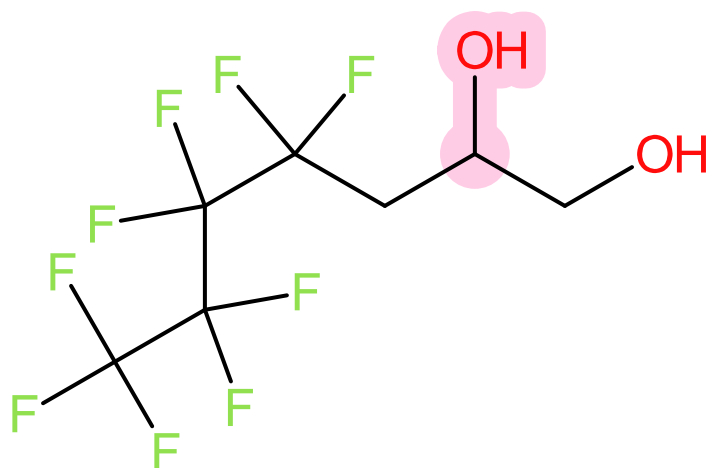
S1: 1-Pentafluoroethylethanol (PFBOH)

SMILES: CC(O)C(F)(F)C(F)(F)F



S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

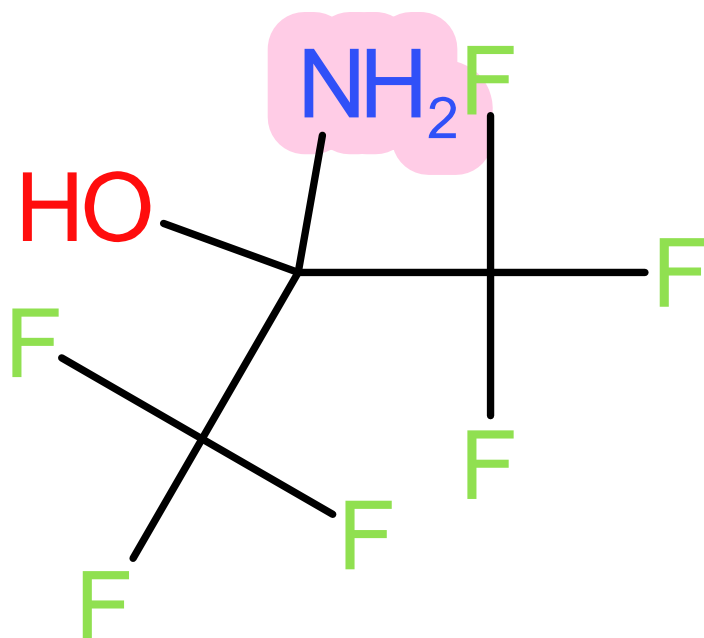
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10343

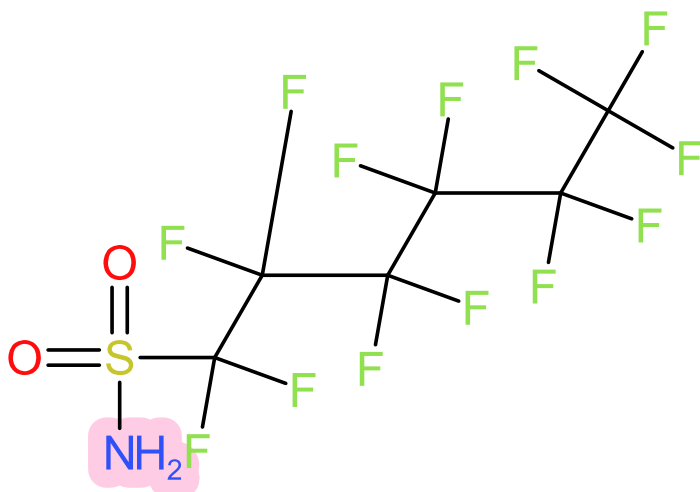
S20: 2-Aminohexafluoropropan-2-ol (AmFPrOH)

SMILES: NC(O)(C(F)(F)F)C(F)(F)F



S31: Perfluorohexanesulfonamide (PFHxSA)

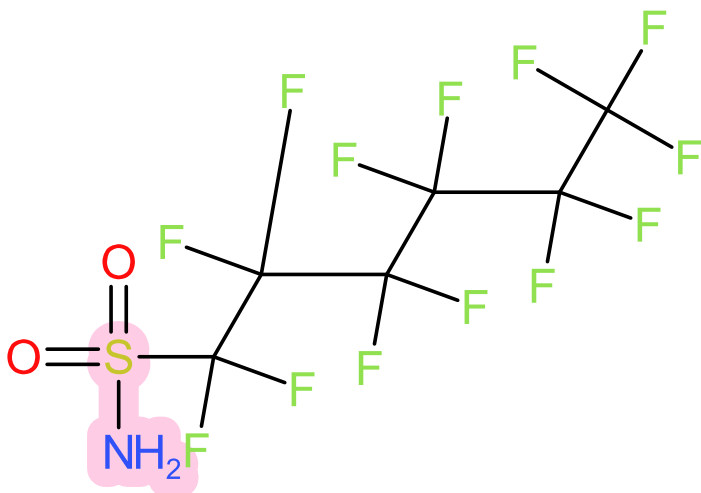
SMILES: NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10099

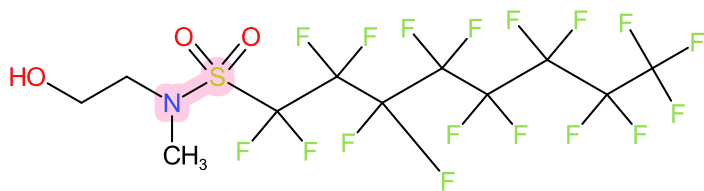
S31: Perfluorohexanesulfonamide (PFHxSA)

SMILES: NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S43: N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide (MeFOSE)

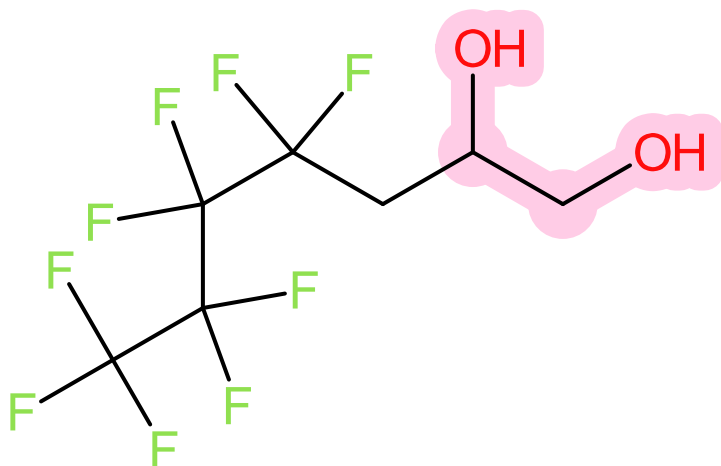
SMILES: CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10289

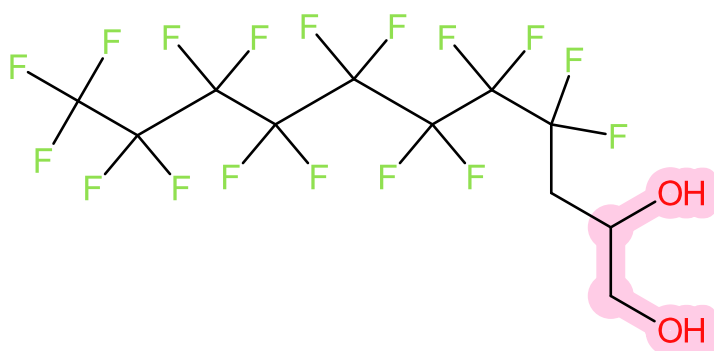
S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S40: 1-(Perfluorooctyl)propane-2,3-diol (PFUd2OH)

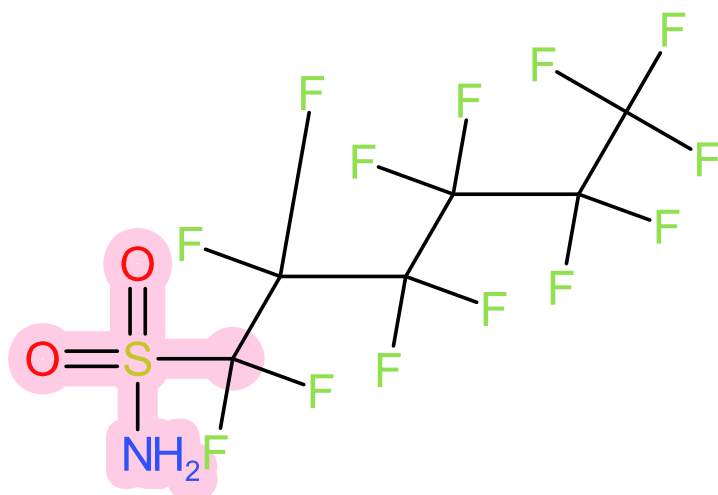
SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



SGR10587

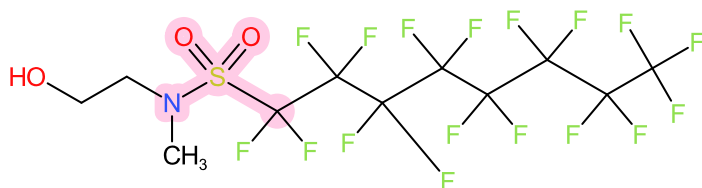
S31: Perfluorohexanesulfonamide (PFHxSA)

SMILES: NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S43: N-Methyl-N-(2-hydroxyethyl)perfluorooctanesulfonamide (MeFOSE)

SMILES: CN(CCO)S(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



TOPOLOGY

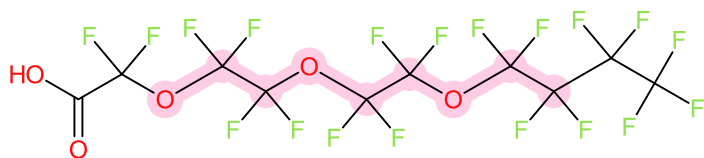
SGR10704 (2 chem)

SGR10749 (2 chem)

SGR10704

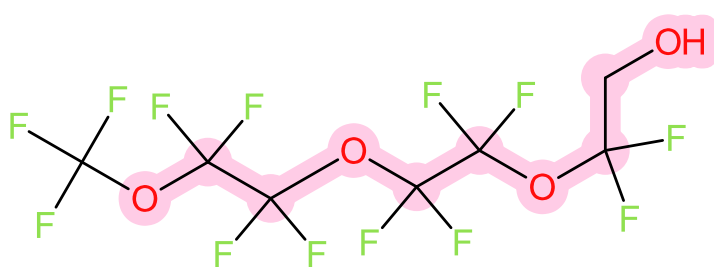
S22: Perfluoro-3,6,9-trioxatridecanoic acid (PFPE-6)

SMILES: OC(=O)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S56: Fluorinated triethylene glycol monomethyl ether (C7F3ETOH)

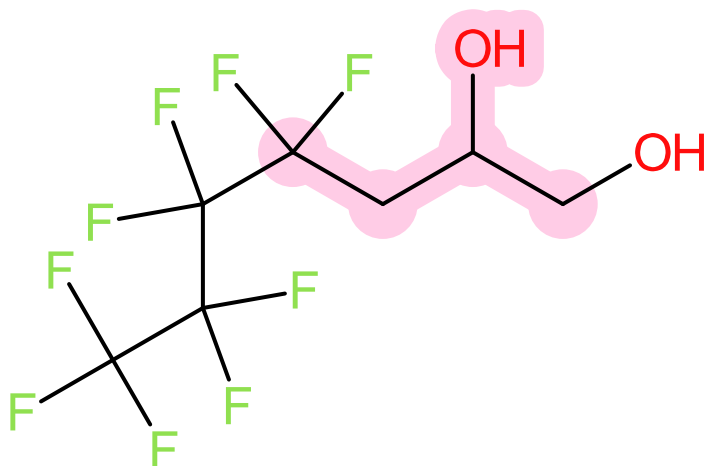
SMILES: OCC(F)(F)OC(F)(F)C(F)(F)OC(F)(F)C(F)(F)OC(F)(F)F



SGR10749

S2: 3-(Perfluoro-2-butyl)propane-1,2-diol (PFHp2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F



S40: 1-(Perfluorooctyl)propane-2,3-diol (PFUd2OH)

SMILES: OCC(O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

