Suppl. Figure 1. Using the prediction algorithm SuperPred we identified dilazep, a vasodilator, as a clinically available drug with potential inhibitory activity against GATA-2

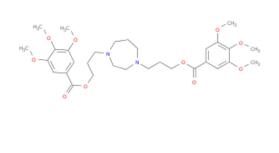
Input structure: K-7174



Information input structure

Name	1,4-bis[(4E)-5-(3,4,5-trimethoxyphenyl)pent-4-en-1-yl]-1,4-diazepane
	→
Formula	C ₃₃ H ₄₈ N ₂ O ₆
Molweight	568.744
xlogP	5.909
Heavy Atoms	41
Rotatable Bonds	16
H-bond Donors	0
H-bond Acceptors	8
Bonds	43
Rings	3
Polar Surface Area	61.860
Total Charge	0

Most similar drug



Drug properties

Name	Dilazep
	4
Formula	C ₃₁ H ₄₄ N ₂ O ₁₀
Molweight	604.688
logP	3.416
Heavy Atoms	43
Rotatable Bonds	18
H-bond Donors	0
H-bond Acceptors	12
Bonds	45
Rings	3
Polar Surface Area	114.46
Total Charge	0