

Astemizole

Inchi:	InChI=1S/C28H31FN4O/c1-34-25-12-8-21(9-13-25)14-17-32-18-15-24(16-19-32)30-28-3
InchiKey:	GXDALQBWZGODGZ-UHFFFAOYSA-N
Formula:	C28H31FN4O
SMILES:	COc1ccc(CCN2CCC(Nc3nc4ccccc4n3Cc3ccc(F)cc3)CC2)cc1
Mol. weight [g/mol]:	458.58
CAS:	68844-77-9

Physical Properties

Property code	Value	Unit	Source
logp	5.351		Crippen Method
mcvol	355.640	ml/mol	McGowan Method
tf	422.20	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/103-351-7/Astemizole.pdf>

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