

Pipamazine

Inchi:	InChI=1S/C21H24ClN3OS/c22-16-6-7-20-18(14-16)25(17-4-1-2-5-19(17)27-20)11-3-10-2
InchiKey:	OSJJYEUEJRVVOD-UHFFFAOYSA-N
Formula:	C21H24ClN3OS
SMILES:	NC(=O)C1CCN(CCCN2c3ccccc3Sc3ccc(Cl)cc32)CC1
Mol. weight [g/mol]:	401.95
CAS:	84-04-8

Physical Properties

Property code	Value	Unit	Source
ie	7.15 ± 0.10	eV	NIST Webbook
log10ws	-5.30		Crippen Method
logp	4.530		Crippen Method
mcvol	297.610	ml/mol	McGowan Method
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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