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