

Clopentixol M (N-oxide)

Inchi: InChI=1S/C22H25ClN2O2S/c23-17-7-8-22-20(16-17)18(19-4-1-2-6-21(19)28-22)5-3-12-2
InchiKey: DTWMRTICXHHUHB-DVZOWYKESA-N
Formula: C22H25ClN2O2S
SMILES: [O-][N+]1(CCC=C2c3ccccc3Sc3ccc(Cl)cc32)CCN(CCO)CC1
Mol. weight [g/mol]: 416.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	4.249		Crippen Method
mcvol	307.590	ml/mol	McGowan Method
rinpola	2409.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R212294&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/32-874-6/Clopentixol-M-N-oxide.pdf>

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