

Tipepidine

Inchi: InChI=1S/C15H17NS2/c1-16-8-2-5-12(11-16)15(13-6-3-9-17-13)14-7-4-10-18-14/h3-4,6-
InchiKey: JWIXXNLOKOOAAQT-UHFFFAOYSA-N
Formula: C15H17NS2
SMILES: CN1CCCC(=C(c2cccs2)c2cccs2)C1
Mol. weight [g/mol]: 275.43
CAS: 5169-78-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	4.337		Crippen Method
mcvol	210.810	ml/mol	McGowan Method
rinpola	2053.00		NIST Webbook
rinpola	2053.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5169788&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

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<https://www.chemeo.com/cid/45-495-3/Tipepidine.pdf>

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