

Dosulepin-M (N-oxide)-(CH3)2NOH

Inchi: InChI=1S/C19H21NOS/c1-20(2,21)13-7-11-17-16-9-4-3-8-15(16)14-22-19-12-6-5-10-18(20)
InchiKey: VYCURIRPXIELFE-BOPFTXTBSA-N
Formula: C19H21NOS
SMILES: C[N+](C)([O-])CCC=C1c2ccccc2CSc2ccccc21
Mol. weight [g/mol]: 311.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	4.688		Crippen Method
mcvol	248.090	ml/mol	McGowan Method
rinsol	2100.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279311&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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