

piperylon

Inchi: InChI=1S/C17H23N3O/c1-3-15-16(13-7-5-4-6-8-13)18-20(17(15)21)14-9-11-19(2)12-10-
InchiKey: LBFQQUCAQWAFNN-UHFFFAOYSA-N
Formula: C17H23N3O
SMILES: CCc1c(-c2ccccc2)[nH]n(C2CCN(C)CC2)c1=O
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	2.191		Crippen Method
mcvol	232.120	ml/mol	McGowan Method
rinpol	2300.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2300.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R211211&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/48-451-8/piperylon.pdf>

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