

Cyprodinil

Inchi: InChI=1S/C14H21N3/c1-10-9-13(11-7-8-11)17-14(15-10)16-12-5-3-2-4-6-12/h9,11-12H,2
InchiKey: BBJFLWKXDDWINV-UHFFFAOYSA-N
Formula: C14H21N3
SMILES: Cc1cc(C2CC2)nc(NC2CCCCC2)n1
Mol. weight [g/mol]: 231.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.407		Crippen Method
mcvol	192.580	ml/mol	McGowan Method
rinpol	2073.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R626970&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/82-642-8/Cyprodinil.pdf>

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