

Norpropyphenazone

Inchi: InChI=1S/C13H16N2O/c1-9(2)12-10(3)14-15(13(12)16)11-7-5-4-6-8-11/h4-9,14H,1-3H3
InchiKey: JEROJODGMFWEEA-UHFFFAOYSA-N
Formula: C13H16N2O
SMILES: Cc1[nH]n(-c2ccccc2)c(=O)c1C(C)C
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.116		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R18222&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/120-908-0/Norpropyphenazone.pdf>

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