

2,3,4,6,7,8,9,10-Octahydro-1H-cyclohepta[d]pyrido

Inchi: InChI=1S/C13H18N2O/c16-13-10-6-2-1-3-7-11(10)14-12-8-4-5-9-15(12)13/h1-9H2
InchiKey: PWJYNQKMHCJCIQH-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: O=c1c2c(nc3n1CCCC3)CCCCC2
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	1.849		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R318337&Units=SI>

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/68-737-9/2-3-4-6-7-8-9-10-Octahydro-1H-cyclohepta-d-pyrido-1-2-a-pyrimidin-11-one.p>

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