

Lophophorine

Inchi: InChI=1S/C13H17NO3/c1-8-11-9(4-5-14(8)2)6-10(15-3)12-13(11)17-7-16-12/h6,8H,4-5,7
InchiKey: PNFBXEKHLUDPIM-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: COc1cc2c(c3c1OCO3)C(C)N(C)CC2
Mol. weight [g/mol]: 235.28
CAS: 17627-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	1.973		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		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=C17627780&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/122-514-5/Lophophorine.pdf>

Generated by Cheméo on 2024-05-01 00:55:47.419799869 +0000 UTC m=+16814196.340377182.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.