

9-(2-Methylbutyryl)platynecine

Other names: 9-(2-Methylbutyryl) platynecine
Inchi: InChI=1S/C13H23NO3/c1-3-9(2)13(16)17-8-10-4-6-14-7-5-11(15)12(10)14/h9-12,15H,3-
InchiKey: JDZNNMHSMYUKBP-YECOWLKZSA-N
Formula: C13H23NO3
SMILES: CCC(C)C(=O)OCC1CCN2CCC(O)C12
Mol. weight [g/mol]: 241.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	1.031		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R395245&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.cheméo.com/cid/40-721-6/9-2-Methylbutylryl-platynecine.pdf>

Generated by Cheméo on 2024-04-19 18:19:11.902244575 +0000 UTC m=+15840000.822821891.

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