

7-(2-Methylbutyryl) platinecine

Other names: 7-(2-Methylbutylryl)platynecine
Inchi: InChI=1S/C13H23NO3/c1-3-9(2)13(16)17-11-5-7-14-6-4-10(8-15)12(11)14/h9-12,15H,3-
InchiKey: BLJYOJVMGNFNQW-YECOWLKZSA-N
Formula: C13H23NO3
SMILES: CCC(C)C(=O)OC1CCN2CCC(CO)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	1778.00		NIST Webbook
rinpol	1778.00		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=R395230&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

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<https://www.chemeo.com/cid/36-059-7/7-2-Methylbutyryl-platinecine.pdf>

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