

13-isobutyryloxylupanine

Inchi: InChI=1S/C19H30N2O3/c1-12(2)19(23)24-15-6-7-20-10-13-8-14(17(20)9-15)11-21-16(13)
InchiKey: FOPGUSZPKIVDDA-WALXCBACSA-N
Formula: C19H30N2O3
SMILES: CC(C)C(=O)OC1CCN2C[C@H]3C[C@@H](CN4C(=O)CCCC34)[C@H]2C1
Mol. weight [g/mol]: 334.46

Physical Properties

Property code	Value	Unit	Source
logp	2.049		Crippen Method
mcvol	264.100	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R390260&Units=SI>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/76-966-6/13-isobutyryloxylupanine.pdf>

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