

1-(Piperidin-1-yl)octadecan-1-one

Inchi: InChI=1S/C23H45NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-17-20-23(25)24-21-18-16-1
InchiKey: MFZHIRGDMBVSTF-UHFFFAOYSA-N
Formula: C23H45NO
SMILES: CCCCCCCCCCCCCCCCCC(=O)N1CCCCC1
Mol. weight [g/mol]: 351.61
CAS: 4629-04-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.69		Crippen Method
logp	7.260		Crippen Method
mcvol	335.620	ml/mol	McGowan Method
rinpol	2841.20		NIST Webbook
rinpol	2841.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4629043&Units=SI>
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>

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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