

(E)-1-(Piperidin-1-yl)octadec-5-en-1-one

Inchi: InChI=1S/C23H43NO/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: FLVOFARNHOWPTO-BUHFOSPRSA-N
Formula: C23H43NO
SMILES: CCCCCCCCCCCC=CCCCC(=O)N1CCCCC1
Mol. weight [g/mol]: 349.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.54		Crippen Method
logp	7.036		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
rinpol	2806.90		NIST Webbook
rinpol	2806.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U412536&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

Latest version available from:

<https://www.chemeo.com/cid/88-541-4/E-1-Piperidin-1-yl-octadec-5-en-1-one.pdf>

Generated by Cheméo on 2024-05-14 09:25:09.098456569 +0000 UTC m=+17967958.019033882.

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