1-(Piperidin-1-yl)dodecan-1-one

Inchi: InChI=1S/C17H33NO/c1-2-3-4-5-6-7-8-9-11-14-17(19)18-15-12-10-13-16-18/h2-16H2,1H
InchiKey: FGQSEPCQVURWHV-UHFFFAOYSA-N
Formula: C17H33NO
SMILES: CCCCCCCCCCCC(=O)N1CCCCC1
Mol. weight [g/mol]: 267.45
CAS: 22342-28-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.920		Crippen Method
mcvol	251.080	ml/mol	McGowan Method
rinpol	2200.60		NIST Webbook
rinpol	2183.00		NIST Webbook
rinpol	2200.60		NIST Webbook
rinpol	2183.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22342285&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices