

1-(Piperidin-1-yl)decan-1-one

Inchi: InChI=1S/C15H29NO/c1-2-3-4-5-6-7-9-12-15(17)16-13-10-8-11-14-16/h2-14H2,1H3
InchiKey: PWSPQJILWCTPAW-UHFFFAOYSA-N
Formula: C15H29NO
SMILES: CCCCCCCCCC(=O)N1CCCCC1
Mol. weight [g/mol]: 239.40
CAS: 5299-66-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	4.140		Crippen Method
mcvol	222.900	ml/mol	McGowan Method
rinpole	1986.50		NIST Webbook
rinpole	1986.50		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5299661&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

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