

Hexadecanoic acid, pyrrolidide

Other names: 1-Hexadecanoylpyrrolidine
Inchi: InChI=1S/C20H39NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20(22)21-18-15-16-19-21/h2
InchiKey: ULDNZNZTSYZQKK-UHFFFAOYSA-N
Formula: C₂₀H₃₉NO
SMILES: CCCCCCCCCCCCCCCCC(=O)N1CCCC1
Mol. weight [g/mol]: 309.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	6.090		Crippen Method
mcvol	293.350	ml/mol	McGowan Method
rinsol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U336152&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemo.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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemo.com/cid/87-492-0/Hexadecanoic-acid-pyrrolidide.pdf>

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