

Isobutyramide, N-tetradecyl-

Inchi: InChI=1S/C18H37NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-18(20)17(2)3/h17H,4-16H
InchiKey: YMRBIHSPBRJWSV-UHFFFAOYSA-N
Formula: C18H37NO
SMILES: CCCCCCCCCCCCCCN=C(O)C(C)C
Mol. weight [g/mol]: 283.49

Physical Properties

Property code	Value	Unit	Source
hf	-499.93	kJ/mol	Joback Method
hvap	75.35	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	6.300		Crippen Method
mcvol	276.030	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
tb	779.54	K	Joback Method
tc	959.62	K	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407099&Units=SI>

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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