Isobutyramide, N-octyl-

Inchi: InChI=1S/C12H25NO/c1-4-5-6-7-8-9-10-13-12(14)11(2)3/h11H,4-10H2,1-3H3,(H,13,14)
InchiKey: WHFDDNBWVNJXEO-UHFFFAOYSA-N
Formula: C12H25NO
SMILES: CCCCCCCCN=C(O)C(C)C
Mol. weight [g/mol]: 199.33

Physical Properties

Property code	Value	Unit	Source
hf	-376.09	kJ/mol	Joback Method
hvap	61.99	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.959		Crippen Method
mcvol	191.490	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
tb	642.26	K	Joback Method
tc	818.86	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407094&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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