

Isobutyramide, N-nonyl-

Inchi: InChI=1S/C13H27NO/c1-4-5-6-7-8-9-10-11-14-13(15)12(2)3/h12H,4-11H2,1-3H3,(H,14,15)1
InchiKey: OKMMHLSMOHODKD-UHFFFAOYSA-N
Formula: C13H27NO
SMILES: CCCCCCCCCN=C(O)C(C)C
Mol. weight [g/mol]: 213.36

Physical Properties

Property code	Value	Unit	Source
hf	-396.73	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.349		Crippen Method
mcvol	205.580	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	665.14	K	Joback Method
tc	841.11	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=U407095&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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