Isobutyramide, N-decyl-

Inchi: InChI=1S/C14H29NO/c1-4-5-6-7-8-9-10-11-12-15-14(16)13(2)3/h13H,4-12H2,1-3H3,(H,1
InchiKey: OJTJXASPLBMSDI-UHFFFAOYSA-N
Formula: C14H29NO
SMILES: CCCCCCCCCCN=C(O)C(C)C
Mol. weight [g/mol]: 227.39

Physical Properties

Property code	Value	Unit	Source
hf	-417.37	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.740		Crippen Method
mcvol	219.670	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
tb	688.02	K	Joback Method
tc	863.77	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407096&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