Isobutyramide, N-undecyl-

Inchi: InChI=1S/C15H31NO/c1-4-5-6-7-8-9-10-11-12-13-16-15(17)14(2)3/h14H,4-13H2,1-3H3,(
InchiKey: DVSGDXNEXBGSJS-UHFFFAOYSA-N
Formula: C15H31NO
SMILES: CCCCCCCCCCCN=C(O)C(C)C
Mol. weight [g/mol]: 241.41

Physical Properties

Property code	Value	Unit	Source
hf	-438.01	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	5.130		Crippen Method
mcvol	233.760	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	710.90	K	Joback Method
tc	886.90	K	Joback Method

Sources

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=U407097&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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