

Isobutyramide, N-(2-ethylhexyl)-

Inchi:	InChI=1S/C12H25NO/c1-5-7-8-11(6-2)9-13-12(14)10(3)4/h10-11H,5-9H2,1-4H3,(H,13,14)
InchiKey:	APULSUCKABFBNS-UHFFFAOYSA-N
Formula:	C12H25NO
SMILES:	CCCCC(CC)CN=C(O)C(C)C
Mol. weight [g/mol]:	199.33

Physical Properties

Property code	Value	Unit	Source
hf	-381.37	kJ/mol	Joback Method
hvap	61.60	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.815		Crippen Method
mcvol	191.490	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
tb	641.82	K	Joback Method
tc	821.11	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407092&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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