Isobutyramide, N-(3-methylbutyl)-

Inchi: InChI=1S/C9H19NO/c1-7(2)5-6-10-9(11)8(3)4/h7-8H,5-6H2,1-4H3,(H,10,11)
InchiKey: YRSZXRYXYXYJAU-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CC(C)CCN=C(O)C(C)C
Mol. weight [g/mol]: 157.25

Physical Properties

Property code	Value	Unit	Source
hf	-319.45	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.645		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1253.00		NIST Webbook
rinpol	1253.00		NIST Webbook
tb	573.18	K	Joback Method
tc	757.00	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=U407088&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