

Isobutyramide, N-pentyl-

Inchi:	InChI=1S/C9H19NO/c1-4-5-6-7-10-9(11)8(2)3/h8H,4-7H2,1-3H3,(H,10,11)
InchiKey:	NFVUCXAYVQLROT-UHFFFAOYSA-N
Formula:	C9H19NO
SMILES:	CCCCCN=C(O)C(C)C
Mol. weight [g/mol]:	157.25

Physical Properties

Property code	Value	Unit	Source
hf	-314.17	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.789		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	573.62	K	Joback Method
tc	754.08	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=U407089&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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