

Valeramide, 5-chloro-N-isobutyl-

Inchi: InChI=1S/C9H18ClNO/c1-8(2)7-11-9(12)5-3-4-6-10/h8H,3-7H2,1-2H3,(H,11,12)
InchiKey: KVQOKZTZOQQPQT-UHFFFAOYSA-N
Formula: C9H18ClNO
SMILES: CC(C)CN=C(O)CCCCCl
Mol. weight [g/mol]: 191.70

Physical Properties

Property code	Value	Unit	Source
hf	-329.91	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	3.008		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1572.00		NIST Webbook
rinpol	1572.00		NIST Webbook
tb	611.05	K	Joback Method
tc	795.95	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407530&Units=SI>
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>

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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