Valeramide, 5-chloro-N-methyl-

Inchi: InChI=1S/C6H12ClNO/c1-8-6(9)4-2-3-5-7/h2-5H2,1H3,(H,8,9)
InchiKey: WXKAAQLKLIQGAO-UHFFFAOYSA-N
Formula: C6H12ClNO
SMILES: CN=C(O)CCCCCl
Mol. weight [g/mol]: 149.62

Physical Properties

Property code	Value	Unit	Source
hf	-262.71	kJ/mol	Joback Method
hvap	53.41	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.982		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
tb	542.85	K	Joback Method
tc	730.26	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=U407528&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