Valeramide, 5-chloro-N-heptyl-

Inchi: InChI=1S/C12H24ClNO/c1-2-3-4-5-8-11-14-12(15)9-6-7-10-13/h2-11H2,1H3,(H,14,15)
InchiKey: ZBRRTJYSGRPGFO-UHFFFAOYSA-N
Formula: C12H24ClNO
SMILES: CCCCCCCN=C(O)CCCCCl
Mol. weight [g/mol]: 233.78

Physical Properties

Property code	Value	Unit	Source
hf	-386.55	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	4.322		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	680.13	K	Joback Method
tc	858.78	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=U407537&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