Valeramide, 5-chloro-N-hexyl-

Inchi: InChI=1S/C11H22ClNO/c1-2-3-4-7-10-13-11(14)8-5-6-9-12/h2-10H2,1H3,(H,13,14)
InchiKey: BAELMQSEJPMTLE-UHFFFAOYSA-N
Formula: C11H22ClNO
SMILES: CCCCCCNC(=O)CCCCCl
Mol. weight [g/mol]: 219.75

Physical Properties

Property code	Value	Unit	Source
gf	-9.72	kJ/mol	Joback Method
hf	-345.22	kJ/mol	Joback Method
hfus	35.14	kJ/mol	Joback Method
hvap	57.65	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.092		Crippen Method
mcvol	189.640	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	592.55	K	Joback Method
tc	771.27	K	Joback Method
tf	346.24	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.67	J/mol×K	592.55	Joback Method
cpg	488.22	J/mol×K	622.34	Joback Method
cpg	502.11	J/mol×K	652.12	Joback Method
cpg	515.33	J/mol×K	681.91	Joback Method
cpg	527.92	J/mol×K	711.70	Joback Method
cpg	539.89	J/mol×K	741.49	Joback Method
cpg	551.26	J/mol×K	771.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407535&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume