Valeramide, 5-chloro-N-(5-chlorovaleryl)-N-propyl-

Inchi: InChI=1S/C13H23Cl2NO2/c1-2-11-16(12(17)7-3-5-9-14)13(18)8-4-6-10-15/h2-11H2,1H3

InchiKey: JSWOESKKUPNKHZ-UHFFFAOYSA-N

Formula: C13H23Cl2NO2

SMILES: CCCN(C(=O)CCCCCl)C(=O)CCCCCl

Mol. weight [g/mol]: 296.23

Physical Properties

Property code	Value	Unit	Source
gf	-112.34	kJ/mol	Joback Method
hf	-500.76	kJ/mol	Joback Method
hfus	44.04	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.570		Crippen Method
mcvol	231.630	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	691.88	K	Joback Method
tc	876.45	K	Joback Method
tf	428.44	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.60	J/mol×K	691.88	Joback Method
cpg	625.78	J/mol×K	722.64	Joback Method
cpg	639.19	J/mol×K	753.40	Joback Method
cpg	651.86	J/mol×K	784.16	Joback Method
cpg	663.82	J/mol×K	814.92	Joback Method
cpg	675.10	J/mol×K	845.68	Joback Method
cpg	685.74	J/mol×K	876.45	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=U407540&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