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

Inchi: InChI=1S/C12H21Cl2NO2/c1-2-15(11(16)7-3-5-9-13)12(17)8-4-6-10-14/h2-10H2,1H3
InchiKey: FDICVUWDKJOUOM-UHFFFAOYSA-N
Formula: C12H21Cl2NO2
SMILES: CCN(C(=O)CCCCCl)C(=O)CCCCCl
Mol. weight [g/mol]: 282.21

Physical Properties

Property code	Value	Unit	Source
gf	-120.76	kJ/mol	Joback Method
hf	-480.12	kJ/mol	Joback Method
hfus	41.45	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.180		Crippen Method
mcvol	217.540	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2106.00		NIST Webbook
tb	669.00	K	Joback Method
tc	854.62	K	Joback Method
tf	417.17	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.67	J/mol×K	669.00	Joback Method
cpg	572.38	J/mol×K	699.94	Joback Method
cpg	585.33	J/mol×K	730.87	Joback Method
cpg	597.57	J/mol×K	761.81	Joback Method
cpg	609.12	J/mol×K	792.75	Joback Method
cpg	620.01	J/mol×K	823.68	Joback Method
cpg	630.28	J/mol×K	854.62	Joback Method

Sources

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=U407539&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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