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

Inchi: InChI=1S/C15H27Cl2NO2/c1-2-3-8-13-18(14(19)9-4-6-11-16)15(20)10-5-7-12-17/h2-13H
InchiKey: FTOGHIHQBDTCHH-UHFFFAOYSA-N
Formula: C15H27Cl2NO2
SMILES: CCCCCN(C(=O)CCCCCl)C(=O)CCCCCl
Mol. weight [g/mol]: 324.29

Physical Properties

Property code	Value	Unit	Source
gf	-95.50	kJ/mol	Joback Method
hf	-542.04	kJ/mol	Joback Method
hfus	49.22	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.350		Crippen Method
mcvol	259.810	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
tb	737.64	K	Joback Method
tc	921.48	K	Joback Method
tf	450.98	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.10	J/mol×K	737.64	Joback Method
cpg	736.13	J/mol×K	768.28	Joback Method
cpg	750.35	J/mol×K	798.92	Joback Method
cpg	763.78	J/mol×K	829.56	Joback Method
cpg	776.46	J/mol×K	860.20	Joback Method
cpg	788.43	J/mol×K	890.84	Joback Method
cpg	799.72	J/mol×K	921.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407543&Units=SI
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

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