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

Inchi: InChI=1S/C11H19Cl2NO2/c1-14(10(15)6-2-4-8-12)11(16)7-3-5-9-13/h2-9H2,1H3
InchiKey: WKRJIWWEFMBRLZ-UHFFFAOYSA-N
Formula: C11H19Cl2NO2
SMILES: CN(C(=O)CCCCCl)C(=O)CCCCCl
Mol. weight [g/mol]: 268.18

Physical Properties

Property code	Value	Unit	Source
gf	-129.18	kJ/mol	Joback Method
hf	-459.48	kJ/mol	Joback Method
hfus	38.86	kJ/mol	Joback Method
hvap	64.39	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.790		Crippen Method
mcvol	203.450	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2103.00		NIST Webbook
tb	646.12	K	Joback Method
tc	833.19	K	Joback Method
tf	405.90	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.07	J/mol×K	646.12	Joback Method
cpg	520.25	J/mol×K	677.30	Joback Method
cpg	532.70	J/mol×K	708.48	Joback Method
cpg	544.46	J/mol×K	739.66	Joback Method
cpg	555.56	J/mol×K	770.83	Joback Method
cpg	566.02	J/mol×K	802.01	Joback Method
cpg	575.87	J/mol×K	833.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407538&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