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

Inchi: InChI=1S/C14H25Cl2NO2/c1-12(2)11-17(13(18)7-3-5-9-15)14(19)8-4-6-10-16/h12H,3-11

InchiKey: RETMFOIPBFYLHW-UHFFFAOYSA-N

Formula: C14H25Cl2NO2

SMILES: CC(C)CN(C(=O)CCCCCl)C(=O)CCCCCl

Mol. weight [g/mol]: 310.26

Physical Properties

Property code	Value	Unit	Source
gf	-106.36	kJ/mol	Joback Method
hf	-526.68	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	70.67	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.816		Crippen Method
mcvol	245.720	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	714.32	K	Joback Method
tc	900.64	K	Joback Method
tf	424.71	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.28	J/mol×K	714.32	Joback Method
cpg	681.11	J/mol×K	745.37	Joback Method
cpg	695.12	J/mol×K	776.43	Joback Method
cpg	708.33	J/mol×K	807.48	Joback Method
cpg	720.79	J/mol×K	838.54	Joback Method
cpg	732.53	J/mol×K	869.59	Joback Method
cpg	743.59	J/mol×K	900.64	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=U407541&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