

Valeramide, 5-chloro-N-(5-chlorovaleryl)-N-(3-methylbutyl)-

Inchi:	InChI=1S/C15H27Cl2NO2/c1-13(2)9-12-18(14(19)7-3-5-10-16)15(20)8-4-6-11-17/h13H,3
InchiKey:	GTACMPFERWBFSC-UHFFFAOYSA-N
Formula:	C15H27Cl2NO2
SMILES:	CC(C)CCN(C(=O)CCCCCl)C(=O)CCCCCl
Mol. weight [g/mol]:	324.29

Physical Properties

Property code	Value	Unit	Source
gf	-97.94	kJ/mol	Joback Method
hf	-547.32	kJ/mol	Joback Method
hfus	45.70	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.206		Crippen Method
mvol	259.810	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	737.20	K	Joback Method
tc	923.14	K	Joback Method
tf	435.98	K	Joback Method
vc	0.998	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.62	J/mol×K	737.20	Joback Method
cpg	736.84	J/mol×K	768.19	Joback Method
cpg	751.22	J/mol×K	799.18	Joback Method
cpg	764.78	J/mol×K	830.17	Joback Method
cpg	777.57	J/mol×K	861.16	Joback Method
cpg	789.62	J/mol×K	892.15	Joback Method
cpg	800.98	J/mol×K	923.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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