Valeramide, 5-chloro-N-octyl-

Inchi: InChI=1S/C13H26ClNO/c1-2-3-4-5-6-9-12-15-13(16)10-7-8-11-14/h2-12H2,1H3,(H,15,16
InchiKey: RDGNMEAMKZMHMK-UHFFFAOYSA-N
Formula: C13H26ClNO
SMILES: CCCCCCCCNC(=O)CCCCCl
Mol. weight [g/mol]: 247.81

Physical Properties

Property code	Value	Unit	Source
gf	7.12	kJ/mol	Joback Method
hf	-386.50	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	62.10	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.872		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	638.31	K	Joback Method
tc	814.69	K	Joback Method
tf	368.78	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.07	J/mol×K	638.31	Joback Method
cpg	592.73	J/mol×K	667.71	Joback Method
cpg	607.65	J/mol×K	697.10	Joback Method
cpg	621.86	J/mol×K	726.50	Joback Method
cpg	635.38	J/mol×K	755.90	Joback Method
cpg	648.24	J/mol×K	785.29	Joback Method
cpg	660.45	J/mol×K	814.69	Joback Method

Sources

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=U407370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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