Valeramide, 5-chloro-N-(2-ethylhexyl)-

Inchi: InChI=1S/C13H26ClNO/c1-3-5-8-12(4-2)11-15-13(16)9-6-7-10-14/h12H,3-11H2,1-2H3,(H
InchiKey: NQNCMKCHFSDKSW-UHFFFAOYSA-N
Formula: C13H26ClNO
SMILES: CCCCC(CC)CNC(=O)CCCCCl
Mol. weight [g/mol]: 247.81

Physical Properties

Property code	Value	Unit	Source
gf	4.68	kJ/mol	Joback Method
hf	-391.78	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	61.71	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.728		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	1933.00		NIST Webbook
rinpol	1933.00		NIST Webbook
tb	637.87	K	Joback Method
tc	816.96	K	Joback Method
tf	353.78	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.49	J/mol×K	637.87	Joback Method
cpg	593.43	J/mol×K	667.72	Joback Method
cpg	608.60	J/mol×K	697.57	Joback Method
cpg	623.03	J/mol×K	727.42	Joback Method
cpg	636.74	J/mol×K	757.27	Joback Method
cpg	649.76	J/mol×K	787.11	Joback Method
cpg	662.12	J/mol×K	816.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407536&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