Hexanamide, 6-chloro-N-ethyl-N-3-methylbutyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	26.07	kJ/mol	Joback Method
hf	-377.72	kJ/mol	Joback Method
hfus	34.72	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.680		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	600.14	K	Joback Method
tc	775.50	K	Joback Method
tf	333.59	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.14	J/mol×K	600.14	Joback Method
cpg	574.72	J/mol×K	629.37	Joback Method
cpg	590.51	J/mol×K	658.59	Joback Method
cpg	605.55	J/mol×K	687.82	Joback Method
cpg	619.85	J/mol×K	717.05	Joback Method
cpg	633.44	J/mol×K	746.27	Joback Method
cpg	646.36	J/mol×K	775.50	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=U415590&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