Hexanamide, 6-chloro-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C12H24ClNO/c1-4-14(10-11(2)3)12(15)8-6-5-7-9-13/h11H,4-10H2,1-3H3
InchiKey: OSOSAQZINRJNMN-UHFFFAOYSA-N
Formula: C12H24ClNO
SMILES: CCN(CC(C)C)C(=O)CCCCCCl
Mol. weight [g/mol]: 233.78

Physical Properties

Property code	Value	Unit	Source
gf	17.65	kJ/mol	Joback Method
hf	-357.08	kJ/mol	Joback Method
hfus	32.13	kJ/mol	Joback Method
hvap	55.09	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.290		Crippen Method
mcvol	203.730	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	577.26	K	Joback Method
tc	753.91	K	Joback Method
tf	322.32	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.50	J/mol×K	577.26	Joback Method
cpg	522.57	J/mol×K	606.70	Joback Method
cpg	537.88	J/mol×K	636.14	Joback Method
cpg	552.45	J/mol×K	665.59	Joback Method
cpg	566.30	J/mol×K	695.03	Joback Method
cpg	579.48	J/mol×K	724.47	Joback Method
cpg	591.99	J/mol×K	753.91	Joback Method

Sources

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=U415588&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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