Hexanamide, 6-chloro-N-ethyl-N-pentyl-

Inchi: InChI=1S/C13H26ClNO/c1-3-5-9-12-15(4-2)13(16)10-7-6-8-11-14/h3-12H2,1-2H3
InchiKey: KVQLCOIPGYTTFW-UHFFFAOYSA-N
Formula: C13H26ClNO
SMILES: CCCCCN(CC)C(=O)CCCCCCl
Mol. weight [g/mol]: 247.81

Physical Properties

Property code	Value	Unit	Source
gf	28.51	kJ/mol	Joback Method
hf	-372.44	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	57.71	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.824		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	600.58	K	Joback Method
tc	773.10	K	Joback Method
tf	348.59	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.78	J/mol×K	600.58	Joback Method
cpg	574.05	J/mol×K	629.33	Joback Method
cpg	589.56	J/mol×K	658.09	Joback Method
cpg	604.34	J/mol×K	686.84	Joback Method
cpg	618.42	J/mol×K	715.59	Joback Method
cpg	631.82	J/mol×K	744.35	Joback Method
cpg	644.57	J/mol×K	773.10	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=U415591&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