Hexanamide, N-ethyl-N-(3-methylphenyl)-6-chloro-

Inchi: InChI=1S/C15H22ClNO/c1-3-17(14-9-7-8-13(2)12-14)15(18)10-5-4-6-11-16/h7-9,12H,3-6
InchiKey: XOQPJEQXXHERBD-UHFFFAOYSA-N
Formula: C15H22ClNO
SMILES: CCN(C(=O)CCCCCCl)c1cccc(C)c1
Mol. weight [g/mol]: 267.79

Physical Properties

Property code	Value	Unit	Source
gf	148.13	kJ/mol	Joback Method
hf	-188.66	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.147		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	678.00	K	Joback Method
tc	879.41	K	Joback Method
tf	410.07	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.50	J/mol×K	678.00	Joback Method
cpg	603.63	J/mol×K	711.57	Joback Method
cpg	618.79	J/mol×K	745.14	Joback Method
cpg	633.02	J/mol×K	778.71	Joback Method
cpg	646.37	J/mol×K	812.28	Joback Method
cpg	658.89	J/mol×K	845.85	Joback Method
cpg	670.61	J/mol×K	879.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308657&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

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