Propanamide, N-ethyl-N-(3-methylphenyl)-3-chloro-

Inchi: InChI=1S/C12H16ClNO/c1-3-14(12(15)7-8-13)11-6-4-5-10(2)9-11/h4-6,9H,3,7-8H2,1-2H

InchiKey: CBHNNONZIXWDRN-UHFFFAOYSA-N

Formula: C12H16ClNO

SMILES: CCN(C(=O)CCCl)c1cccc(C)c1

Mol. weight [g/mol]: 225.72

Physical Properties

Property code	Value	Unit	Source
gf	122.87	kJ/mol	Joback Method
hf	-126.74	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.977		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1683.00		NIST Webbook
rinpol	1683.00		NIST Webbook
tb	609.36	K	Joback Method
tc	819.61	K	Joback Method
tf	376.26	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.86	J/mol×K	609.36	Joback Method
cpg	447.62	J/mol×K	644.40	Joback Method
cpg	461.44	J/mol×K	679.44	Joback Method
cpg	474.38	J/mol×K	714.49	Joback Method
cpg	486.47	J/mol×K	749.53	Joback Method
cpg	497.76	J/mol×K	784.57	Joback Method
cpg	508.29	J/mol×K	819.61	Joback Method

Sources

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=U308501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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