Propanamide, N-ethyl-N-(3-methylphenyl)-2-chloro-

Inchi: InChI=1S/C12H16ClNO/c1-4-14(12(15)10(3)13)11-7-5-6-9(2)8-11/h5-8,10H,4H2,1-3H3
InchiKey: UQTVJWBAWLRDEE-UHFFFAOYSA-N
Formula: C12H16ClNO
SMILES: CCN(C(=O)C(C)Cl)c1cccc(C)c1
Mol. weight [g/mol]: 225.72

Physical Properties

Property code	Value	Unit	Source
gf	120.43	kJ/mol	Joback Method
hf	-132.02	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	58.03	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.975		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1589.00		NIST Webbook
tb	608.92	K	Joback Method
tc	823.46	K	Joback Method
tf	361.26	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.29	J/mol×K	608.92	Joback Method
cpg	448.40	J/mol×K	644.68	Joback Method
cpg	462.53	J/mol×K	680.43	Joback Method
cpg	475.72	J/mol×K	716.19	Joback Method
cpg	488.02	J/mol×K	751.95	Joback Method
cpg	499.48	J/mol×K	787.70	Joback Method
cpg	510.14	J/mol×K	823.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308384&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