Benzamide, N-(3-methylphenyl)-2-chloro-

Inchi: InChI=1S/C14H12ClNO/c1-10-5-4-6-11(9-10)16-14(17)12-7-2-3-8-13(12)15/h2-9H,1H3,(
InchiKey: QMUDBMHUUBUXHG-UHFFFAOYSA-N
Formula: C14H12ClNO
SMILES: Cc1cccc(NC(=O)c2ccccc2Cl)c1
Mol. weight [g/mol]: 245.70

Physical Properties

Property code	Value	Unit	Source
gf	221.10	kJ/mol	Joback Method
hf	42.98	kJ/mol	Joback Method
hfus	30.22	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.901		Crippen Method
mcvol	184.390	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	724.51	K	Joback Method
tc	972.24	K	Joback Method
tf	457.93	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.13	J/mol×K	724.51	Joback Method
cpg	476.46	J/mol×K	765.80	Joback Method
cpg	488.65	J/mol×K	807.09	Joback Method
cpg	499.77	J/mol×K	848.38	Joback Method
cpg	509.90	J/mol×K	889.66	Joback Method
cpg	519.12	J/mol×K	930.95	Joback Method
cpg	527.47	J/mol×K	972.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306979&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