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

Inchi: InChI=1S/C13H9Cl2NO/c14-9-4-3-5-10(8-9)16-13(17)11-6-1-2-7-12(11)15/h1-8H,(H,16,1
InchiKey: HWDAIZBRWARIMB-UHFFFAOYSA-N
Formula: C13H9Cl2NO
SMILES: O=C(Nc1cccc(Cl)c1)c1ccccc1Cl
Mol. weight [g/mol]: 266.12

Physical Properties

Property code	Value	Unit	Source
gf	200.75	kJ/mol	Joback Method
hf	47.88	kJ/mol	Joback Method
hfus	31.82	kJ/mol	Joback Method
hvap	72.36	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.246		Crippen Method
mcvol	182.540	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	739.06	K	Joback Method
tc	994.35	K	Joback Method
tf	476.58	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.96	J/mol×K	739.06	Joback Method
cpg	445.49	J/mol×K	781.61	Joback Method
cpg	455.93	J/mol×K	824.16	Joback Method
cpg	465.38	J/mol×K	866.71	Joback Method
cpg	473.90	J/mol×K	909.26	Joback Method
cpg	481.57	J/mol×K	951.80	Joback Method
cpg	488.47	J/mol×K	994.35	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306980&Units=SI

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