Formamide, N-(2-chlorophenyl)-

Other names: Formanilide, 2'-chloro-
2'-Chloroformanilide
Inchi: InChI=1S/C7H6ClNO/c8-6-3-1-2-4-7(6)9-5-10/h1-5H,(H,9,10)
InchiKey: DGRDTMLQUWBPSM-UHFFFAOYSA-N
Formula: C7H6ClNO
SMILES: O=CNc1ccccc1Cl
Mol. weight [g/mol]: 155.58
CAS: 2596-93-2

Physical Properties

Property code	Value	Unit	Source
gf	88.78	kJ/mol	Joback Method
hf	-10.60	kJ/mol	Joback Method
hfus	19.12	kJ/mol	Joback Method
hvap	51.66	kJ/mol	Joback Method
ie	8.40 ± 0.10	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.908		Crippen Method
mcvol	109.520	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	527.48	K	Joback Method
tc	754.60	K	Joback Method
tf	332.17	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.72	J/mol×K	527.48	Joback Method
cpg	226.18	J/mol×K	565.33	Joback Method
cpg	234.98	J/mol×K	603.19	Joback Method
cpg	243.15	J/mol×K	641.04	Joback Method
cpg	250.72	J/mol×K	678.89	Joback Method
cpg	257.71	J/mol×K	716.75	Joback Method

cpg	264.16	J/mol×K	754.60	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=C2596932&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume