o-Chloroacetanilide

Other names:	2'-Chloro acetanilide
	2-Chloroacetanilide
	Acetamide, N-(2-chlorophenyl)-
	Acetanilide, 2'-chloro-
	N-(2-Chlorophenyl)acetamide
Inchi:	InChI=1S/C8H8ClNO/c1-6(11)10-8-5-3-2-4-7(8)9/h2-5H,1H3,(H,10,11)
InchiKey:	KNVQTRVKSOEHPU-UHFFFAOYSA-N
Formula:	C8H8ClNO
SMILES:	CC(=O)Nc1ccccc1Cl
Mol. weight [g/mol]:	169.61
CAS:	533-17-5

Physical Properties

Property code	Value	Unit	Source
gf	67.80	kJ/mol	Joback Method
hf	-58.24	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
ie	8.07 ± 0.03	eV	NIST Webbook
ie	8.55	eV	NIST Webbook
log10ws	-1.40		Aqueous Solubility Prediction Method
logp	2.298		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	3759.17	kPa	Joback Method
tb	555.57	K	Joback Method
tc	784.08	K	Joback Method
tf	359.90 ± 0.50	K	NIST Webbook
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.93	J/mol×K	555.57	Joback Method

cpg	268.79	J/mol×K	593.65	Joback Method
cpg	278.91	J/mol×K	631.74	Joback Method
cpg	288.31	J/mol×K	669.82	Joback Method
cpg	297.04	J/mol×K	707.91	Joback Method
cpg	305.11	J/mol×K	745.99	Joback Method
cpg	312.56	J/mol×K	784.08	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C533175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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