Acetamide, N-(4-chlorophenyl)-

Other names:	4'-Chloroacetanilide
	4-Chloroacetanilide
	Acet-p-chloroanilide
	Acetanilide, 4'-chloro-
	Acetic acid-4-chloroanilide
	Acetic-4-chloroanilide
	N(4-chlorophenyl)ethanamide
	N-(4-Chlorophenyl)acetamide
	N-(p-Chlorophenyl)acetamide
	N-Acetyl-4-chloroaniline
	N-Acetyl-p-chloroaniline
	NSC 40563
	ethanamide, N(4-chlorophenyl)-
	p-Chloroacetanilide
	p-Chloroacetoanilide
	para-chloroacetanilide
Inchi:	InChI=1S/C8H8ClNO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)
InchiKey:	GGUOCFNAWIODMF-UHFFFAOYSA-N
Formula:	C8H8ClNO
SMILES:	CC(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]:	169.61
CAS:	539-03-7

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	8.30 ± 0.20	eV	NIST Webbook
log10ws	-2.84		Aqueous Solubility Prediction Method
log10ws	-2.84		Estimated Solubility 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	451.60 ± 0.50	K	NIST Webbook
tf	448.80	K	Thermodynamic properties of paracetamol impurities 4-nitrophenol and 4'-chloroacetanilide and the impact of such impurities on the crystallisation of paracetamol from solution
tf	451.82	K	Aqueous Solubility Prediction Method
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

Thermodynamic properties of paracetamol impurities 4-nitrophenol and 4'-chloroacetanilide and the impact of such impurities on the crystallisation of paracetamol from solution:	https://www.doi.org/10.1016/j.jct.2019.02.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C539037&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