Acetamide, N-(3-chlorophenyl)-

Other names:	Acetanilide, 3'-chloro-
	m-Chloroacetanilide
	3-Chloroacetanilide
	3'-Chloroacetanilide
	N-(3-Chlorophenyl)acetic acid amide
Inchi:	InChI=1S/C8H8ClNO/c1-6(11)10-8-4-2-3-7(9)5-8/h2-5H,1H3,(H,10,11)
InchiKey:	MUUQHCOAOLLHIL-UHFFFAOYSA-N
Formula:	C8H8ClNO
SMILES:	CC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]:	169.61
CAS:	588-07-8

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	8.70 ± 0.20	eV	NIST Webbook
log10ws	-2.36		Crippen 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	349.80 ± 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C588078&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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