Acetamide, N-(2,6-dichlorophenyl)-

Other names:	Acetanilide, 2',6'-dichloro-
	2,6-Dichloroacetanilide
	2',6'-Dichloroacetanilide
	N-(2,6-dichlorophenyl)acetamide
Inchi:	InChI=1S/C8H7Cl2NO/c1-5(12)11-8-6(9)3-2-4-7(8)10/h2-4H,1H3,(H,11,12)
InchiKey:	DWVWVSLAIJHBBG-UHFFFAOYSA-N
Formula:	C8H7Cl2NO
SMILES:	CC(=O)Nc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	204.05
CAS:	17700-54-8

Physical Properties

Property code	Value	Unit	Source
gf	46.24	kJ/mol	Joback Method
hf	-85.45	kJ/mol	Joback Method
hfus	24.83	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
ie	8.25 ± 0.03	eV	NIST Webbook
log10ws	-3.04		Crippen Method
logp	2.952		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	597.98	K	Joback Method
tc	831.44	K	Joback Method
tf	393.81	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.93	J/mol×K	597.98	Joback Method
cpg	288.66	J/mol×K	636.89	Joback Method
cpg	297.69	J/mol×K	675.80	Joback Method
cpg	306.07	J/mol×K	714.71	Joback Method

cpg	313.81	J/mol×K	753.62	Joback Method
cpg	320.94	J/mol×K	792.53	Joback Method
cpg	327.50	J/mol×K	831.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17700548&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