

3',4'-Dichloroacetanilide

Other names:	Acetanilide, 3',4'-dichloro- N-(3,4-Dichlorophenyl)acetamide NSC 30069 N-Acetyl-3,4-dichloroaniline
Inchi:	InChI=1S/C8H7Cl2NO/c1-5(12)11-6-2-3-7(9)8(10)4-6/h2-4H,1H3,(H,11,12)
InchiKey:	SCYGGCAQZFJGRF-UHFFFAOYSA-N
Formula:	C8H7Cl2NO
SMILES:	CC(=O)Nc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	204.05
CAS:	2150-93-8

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
log10ws	-3.04		Crippen Method
logp	2.952		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
rinpol	1727.00		NIST Webbook
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/molxK	597.98	Joback Method
cpg	288.66	J/molxK	636.89	Joback Method
cpg	297.69	J/molxK	675.80	Joback Method
cpg	306.07	J/molxK	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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2150938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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