

2',5'-Dichloro-4'-nitroacetanilide

Other names:	Acetamide, N-(2,5-dichloro-4-nitrophenyl)- Acetanilide, 2',5'-dichloro-4'-nitro- 2,5-Dichlor-4-nitroacetanilid N-(2,5-dichloro-4-nitrophenyl)acetamide
Inchi:	InChI=1S/C8H6Cl2N2O3/c1-4(13)11-7-2-6(10)8(12(14)15)3-5(7)9/h2-3H,1H3,(H,11,13)
InchiKey:	YOKGZPNQGIYATO-UHFFFAOYSA-N
Formula:	C8H6Cl2N2O3
SMILES:	CC(=O)Nc1cc(Cl)c([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]:	249.05
CAS:	38411-17-5

Physical Properties

Property code	Value	Unit	Source
gf	72.16	kJ/mol	Joback Method
hf	-107.68	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.860		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	754.80	K	Joback Method
tc	1009.30	K	Joback Method
tf	549.94	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.24	J/molxK	754.80	Joback Method
cpg	363.53	J/molxK	797.22	Joback Method
cpg	371.04	J/molxK	839.63	Joback Method
cpg	377.82	J/molxK	882.05	Joback Method
cpg	383.89	J/molxK	924.46	Joback Method

cpg	389.31	J/mol×K	966.88	Joback Method
cpg	394.09	J/mol×K	1009.30	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=C38411175&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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