

4,5-Dichloro-ortho-phenylenediamine

Other names:	4,5-Dichloro-1,2-phenylenediamine 4,5-Dichloro-o-phenylenediamine 1,2-Benzenediamine, 4,5-dichloro-o-Phenylenediamine, 4,5-dichloro-1,2-Diamino-4,5-dichlorobenzene 1,2-Dichloro-4,5-diaminobenzene 4,5-Dichloro-o-phenylendiamine 4,5-Dichloro-1,2-benzenediamine 2-Amino-4,5-dichloroaniline NSC 1577
Inchi:	InChI=1S/C6H6Cl2N2/c7-3-1-5(9)6(10)2-4(3)8/h1-2H,9-10H2
InchiKey:	IWFHBRFJOHTIPU-UHFFFAOYSA-N
Formula:	C6H6Cl2N2
SMILES:	Nc1cc(Cl)c(Cl)cc1N
Mol. weight [g/mol]:	177.03
CAS:	5348-42-5

Physical Properties

Property code	Value	Unit	Source
gf	192.20	kJ/mol	Joback Method
hf	71.05	kJ/mol	Joback Method
hfus	22.96	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.158		Crippen Method
mcvol	116.080	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
tb	598.22	K	Joback Method
tc	852.55	K	Joback Method
tf	447.72	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.43	J/mol×K	598.22	Joback Method
cpg	242.49	J/mol×K	640.61	Joback Method
cpg	249.97	J/mol×K	683.00	Joback Method
cpg	256.88	J/mol×K	725.39	Joback Method
cpg	263.26	J/mol×K	767.77	Joback Method
cpg	269.12	J/mol×K	810.16	Joback Method
cpg	274.50	J/mol×K	852.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5348425&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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