

Phenol, 4-amino-2,6-dichloro-

Other names:	2,6-Dichloro-p-aminophenol 2,6-Dichloro-4-aminophenol 3,5-Dichloro-4-hydroxyaniline 4-Amino-2,6-dichlorophenol
Inchi:	InChI=1S/C6H5Cl2NO/c7-4-1-3(9)2-5(8)6(4)10/h1-2,10H,9H2
InchiKey:	KGEXISHTCZHGFU-UHFFFAOYSA-N
Formula:	C6H5Cl2NO
SMILES:	Nc1cc(Cl)c(O)c(Cl)c1
Mol. weight [g/mol]:	178.02
CAS:	5930-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-19.24	kJ/mol	Joback Method
hf	-128.58	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.281		Crippen Method
mcvol	111.970	ml/mol	McGowan Method
pc	5398.63	kPa	Joback Method
tb	601.33	K	Joback Method
tc	857.23	K	Joback Method
tf	463.66	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.57	J/molxK	601.33	Joback Method
cpg	234.55	J/molxK	643.98	Joback Method
cpg	240.95	J/molxK	686.63	Joback Method
cpg	246.87	J/molxK	729.28	Joback Method
cpg	252.40	J/molxK	771.93	Joback Method

cpg	257.64	J/mol×K	814.58	Joback Method
cpg	262.67	J/mol×K	857.23	Joback Method

Sources

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=C5930289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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