

1,5-diaminochloro-4,8-dihydroxyanthraquinone

Other names:	1,5-Diaminochloro-4,8-dihydroxyanthraquinone (C.I. disperse blue 56)
Inchi:	InChI=1S/C14H9ClN2O4/c15-5-1-3-7(18)11-9(5)13(20)12-8(19)4-2-6(17-16)10(12)14(11)
InchiKey:	VADWVKWRBQETDP-UHFFFAOYSA-N
Formula:	C14H9ClN2O4
SMILES:	<chem>NNc1ccc(O)c2c1C(=O)c1c(O)ccc(Cl)c1C2=O</chem>
Mol. weight [g/mol]:	304.69
CAS:	12217-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-76.65	kJ/mol	Joback Method
hf	-364.31	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	109.99	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	1.812		Crippen Method
mcvol	196.820	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
tb	1057.15	K	Joback Method
tc	1339.55	K	Joback Method
tf	901.88	K	Joback Method
vc	0.628	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.16	J/mol×K	1057.15	Joback Method
cpg	616.05	J/mol×K	1104.22	Joback Method
cpg	629.46	J/mol×K	1151.28	Joback Method
cpg	643.60	J/mol×K	1198.35	Joback Method
cpg	658.69	J/mol×K	1245.42	Joback Method
cpg	674.93	J/mol×K	1292.48	Joback Method
cpg	692.53	J/mol×K	1339.55	Joback Method
hsubt	93.30	kJ/mol	508.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C12217797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hsubt:	Enthalpy of sublimation at a given temperature
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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