

2,5-Cyclohexadiene-1,4-dione, 2,5-dichloro-3,6-dihydroxy-

Other names:	Chloranilic acid p-Benzoquinone, 2,5-dichloro-3,6-dihydroxy- 2,5-Dihydroxy-3,6-dichlorobenzoquinone 2,5-dichloro-3,6-dihydroxybenzoquinone
Inchi:	InChI=1S/C6H2Cl2O4/c7-1-3(9)5(11)2(8)6(12)4(1)10/h9,12H
InchiKey:	IPPWILKKGXFOXHO-UHFFFAOYSA-N
Formula:	C6H2Cl2O4
SMILES:	O=C1C(O)=C(Cl)C(=O)C(O)=C1Cl
Mol. weight [g/mol]:	208.98
CAS:	87-88-7

Physical Properties

Property code	Value	Unit	Source
chs	-2029.00	kJ/mol	NIST Webbook
gf	-489.48	kJ/mol	Joback Method
hf	-634.17	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	83.54	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.155		Crippen Method
mcvol	115.300	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
tb	774.00	K	Joback Method
tc	996.03	K	Joback Method
tf	538.52	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.91	J/molxK	774.00	Joback Method
cpg	264.73	J/molxK	811.00	Joback Method
cpg	269.99	J/molxK	848.01	Joback Method
cpg	274.65	J/molxK	885.01	Joback Method

cpg	278.65	J/mol×K	922.02	Joback Method
cpg	281.94	J/mol×K	959.02	Joback Method
cpg	284.45	J/mol×K	996.03	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=C87887&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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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