Chloranilic acid

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:	IPPWILKGXFOXHO-UHFFFAOYSA-N
Formula:	C6H2Cl2O4
SMILES:	O=C1C(O)=C(Cl)C(=O)C(O)=C1Cl
Mol. weight [g/mol]:	208.98

Physical Properties

Property code	Value	Unit	Source
chs	-2029.00	kJ/mol	NIST Webbook
hfus	18.54	kJ/mol	Joback Method
ie	9.66	eV	Cheméo Relay (1.0)
logp	1.155		Crippen Method
mcvol	115.300	ml/mol	McGowan Method
tf	474.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87887&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point