Tetroquinone

Other names:	2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrahydroxy- p-Benzoquinone, 2,3,5,6-tetrahydroxy- HPEK-1 Kelox Terasin Tetrahydroxy-p-benzoquinone Tetrahydroxy-p-quinone Tetrahydroxy-1,4-benzoquinone Tetrahydroxyparabenzoquinone Tetrahydroxyquinone THQ 2,3,5,6-Tetrahydroxy-p-benzoquinone Tetrahydroxy-1,4-quinone 2,3,5,6-Tetrahydroxy-2,5-cyclohexadien-1,4-dione NSC-112931
Inchi:	InChI=1S/C6H4O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h7-8,11-12H
InchiKey:	DGQOCLATAPFASR-UHFFFAOYSA-N
Formula:	C6H4O6
SMILES:	O=C1C(O)=C(O)C(=O)C(O)=C1O
Mol. weight [g/mol]:	172.09
CAS:	319-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-739.26	kJ/mol	Joback Method
hf	-907.15	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	108.13	kJ/mol	Joback Method
log10ws	0.23		Crippen Method
logp	-0.207		Crippen Method
mcvol	102.560	ml/mol	McGowan Method
pc	8175.04	kPa	Joback Method
tb	883.50	K	Joback Method
tc	1088.58	K	Joback Method
tf	600.32	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.83	J/mol×K	883.50	Joback Method
cpg	297.33	J/mol×K	917.68	Joback Method
cpg	301.20	J/mol×K	951.86	Joback Method
cpg	304.38	J/mol×K	986.04	Joback Method
cpg	306.83	J/mol×K	1020.22	Joback Method
cpg	308.51	J/mol×K	1054.40	Joback Method
cpg	309.38	J/mol×K	1088.58	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=C319891&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