p-Benzoquinone, 2,3,5,6-tetrafluoro-

Other names:	p-Fluoranil
	2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrafluoro-
	Fluoranil
	Fluoroanil
	Tetrafluoro-p-benzoquinone
	Tetrafluoro-1,4-benzoquinone
	Tetrafluoroquinone
	2,3,5,6-Tetrafluoro-p-benzoquinone
	Perfluoro-p-benzoquinone
	p-Benzoquinone, tetrafluoro-
	2,3,5,6-Tetrafluoro-1,4-benzoquinone
	Tetrafluorobenzoquinone
	NSC 264881
	Tetrafluoro-p-quinone
Inchi:	InChI=1S/C6F4O2/c7-1-2(8)6(12)4(10)3(9)5(1)11
InchiKey:	JKLYZOGJWVAIQS-UHFFFAOYSA-N
Formula:	C6F4O2
SMILES:	O=C1C(F)=C(F)C(=O)C(F)=C1F
Mol. weight [g/mol]:	180.06
CAS:	527-21-9

Physical Properties

Property code	Value	Unit	Source
ea	2.70 ± 0.10	eV	NIST Webbook
ea	2.45 ± 0.05	eV	NIST Webbook
ea	2.92 ± 0.20	eV	NIST Webbook
ea	2.27	eV	NIST Webbook
gf	-971.22	kJ/mol	Joback Method
hf	-1082.67	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	38.15	kJ/mol	Joback Method
ie	10.70	eV	NIST Webbook
ie	10.96 ± 0.05	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.439		Crippen Method
mcvol	86.160	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method

tb	511.86	K	Joback Method
tc	719.14	K	Joback Method
tf	359.40	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.54	J/mol×K	511.86	Joback Method
cpg	191.82	J/mol×K	546.41	Joback Method
cpg	198.99	J/mol×K	580.95	Joback Method
cpg	206.01	J/mol×K	615.50	Joback Method
cpg	212.82	J/mol×K	650.05	Joback Method
cpg	219.37	J/mol×K	684.59	Joback Method
cpg	225.62	J/mol×K	719.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C527219&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
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
ie: Ionization energy
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