Tetrabromo-1,2-benzoquinone

Other names:	Tetrabromo-o-benzoquinone
	o-Bromanil
	3,5-Cyclohexadiene-1,2-dione, 3,4,5,6-tetrabromo-
	3,4,5,6-tetrabromo-o-benzoquinone
Inchi:	InChI=1S/C6Br4O2/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	DXKHBLYQXDEINJ-UHFFFAOYSA-N
Formula:	C6Br4O2
SMILES:	O=C1C(=O)C(Br)=C(Br)C(Br)=C1Br
Mol. weight [g/mol]:	423.68
CAS:	2435-54-3

Physical Properties

Property code	Value	Unit	Source
ea	2.44 ± 0.20	eV	NIST Webbook
gf	-134.70	kJ/mol	Joback Method
hf	-192.91	kJ/mol	Joback Method
hfus	23.11	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.141		Crippen Method
mcvol	149.080	ml/mol	McGowan Method
pc	6967.65	kPa	Joback Method
tb	779.42	K	Joback Method
tc	1086.46	K	Joback Method
tf	596.24	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.69	J/mol×K	779.42	Joback Method
cpg	252.80	J/mol×K	830.59	Joback Method
cpg	258.12	J/mol×K	881.77	Joback Method
cpg	262.60	J/mol×K	932.94	Joback Method

cpg	266.16	J/mol×K	984.12	Joback Method
cpg	268.74	J/mol×K	1035.29	Joback Method
cpg	270.27	J/mol×K	1086.46	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=C2435543&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
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
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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