Me-triCl-p-benzoquinone radical

Inchi: InChI=1S/C7H3Cl3O2/c1-2-3(8)7(12)5(10)4(9)6(2)11/h1H3
InchiKey: ZBWPOKNIKGLQBA-UHFFFAOYSA-N
Formula: C7H3Cl3O2
SMILES: CC1=C(Cl)C(=O)C(Cl)=C(Cl)C1=O
Mol. weight [g/mol]: 225.46
CAS: 4592-97-6

Physical Properties

Property code	Value	Unit	Source
ea	2.54 ± 0.05	eV	NIST Webbook
gf	-219.35	kJ/mol	Joback Method
hf	-366.09	kJ/mol	Joback Method
hfus	17.15	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.340		Crippen Method
mcvol	129.890	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	649.95	K	Joback Method
tc	912.16	K	Joback Method
tf	458.07	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.94	J/mol×K	649.95	Joback Method
cpg	263.21	J/mol×K	693.65	Joback Method
cpg	271.91	J/mol×K	737.35	Joback Method
cpg	279.95	J/mol×K	781.05	Joback Method
cpg	287.25	J/mol×K	824.75	Joback Method
cpg	293.71	J/mol×K	868.46	Joback Method
cpg	299.24	J/mol×K	912.16	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C4592976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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