2-Cl-5-Me-p-benzoquinone radical

Inchi: InChI=1S/C7H5ClO2/c1-4-2-7(10)5(8)3-6(4)9/h2-3H,1H3
InchiKey: BIUBEGIHROOPTQ-UHFFFAOYSA-N
Formula: C7H5ClO2
SMILES: CC1=CC(=O)C(Cl)=CC1=O
Mol. weight [g/mol]: 156.57
CAS: 19832-87-2

Physical Properties

Property code	Value	Unit	Source
ea	2.11 ± 0.05	eV	NIST Webbook
gf	-176.23	kJ/mol	Joback Method
hf	-311.67	kJ/mol	Joback Method
hfus	9.53	kJ/mol	Joback Method
hvap	46.70	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.207		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	565.13	K	Joback Method
tc	819.03	K	Joback Method
tf	373.19	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.82	J/mol×K	565.13	Joback Method
cpg	226.83	J/mol×K	607.45	Joback Method
cpg	237.35	J/mol×K	649.76	Joback Method
cpg	247.31	J/mol×K	692.08	Joback Method
cpg	256.65	J/mol×K	734.40	Joback Method
cpg	265.30	J/mol×K	776.71	Joback Method
cpg	273.18	J/mol×K	819.03	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=C19832872&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