2,5-diCl-3,6-diMe-p-benzoquinone radical

Inchi: InChI=1S/C8H6Cl2O2/c1-3-5(9)8(12)4(2)6(10)7(3)11/h1-2H3
InchiKey: VCJSHLWROQUHPY-UHFFFAOYSA-N
Formula: C8H6Cl2O2
SMILES: CC1=C(Cl)C(=O)C(C)=C(Cl)C1=O
Mol. weight [g/mol]: 205.04
CAS: 46010-98-4

Physical Properties

Property code	Value	Unit	Source
ea	2.23 ± 0.05	eV	NIST Webbook
gf	-199.00	kJ/mol	Joback Method
hf	-370.99	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	54.64	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.164		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	635.40	K	Joback Method
tc	888.85	K	Joback Method
tf	439.42	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.02	J/mol×K	635.40	Joback Method
cpg	291.15	J/mol×K	677.64	Joback Method
cpg	301.68	J/mol×K	719.88	Joback Method
cpg	311.53	J/mol×K	762.13	Joback Method
cpg	320.62	J/mol×K	804.37	Joback Method
cpg	328.87	J/mol×K	846.61	Joback Method
cpg	336.20	J/mol×K	888.85	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C46010984&Units=SI

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