2-chloro-1,4-naphthoquinone

Inchi: InChI=1S/C10H5ClO2/c11-8-5-9(12)6-3-1-2-4-7(6)10(8)13/h1-5H
InchiKey: CCTJHVLTAJTPBV-UHFFFAOYSA-N
Formula: C10H5ClO2
SMILES: O=C1C=C(Cl)C(=O)c2ccccc21
Mol. weight [g/mol]: 192.60
CAS: 1010-60-2

Physical Properties

Property code	Value	Unit	Source
gf	-44.32	kJ/mol	Joback Method
hf	-182.52	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.80 ± 0.02	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	2.188		Crippen Method
mcvol	128.220	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	652.75	K	Joback Method
tc	923.21	K	Joback Method
tf	439.70	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.20	J/mol×K	652.75	Joback Method
cpg	304.38	J/mol×K	697.83	Joback Method
cpg	315.60	J/mol×K	742.90	Joback Method
cpg	325.87	J/mol×K	787.98	Joback Method
cpg	335.15	J/mol×K	833.05	Joback Method
cpg	343.44	J/mol×K	878.13	Joback Method
cpg	350.72	J/mol×K	923.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1010602&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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