2-Chloro-3-methyl-1,4-naphthoquinone

Other names: 2-Chloro-3-methylnaphthoquinone
Inchi: InChI=1S/C11H7ClO2/c1-6-9(12)11(14)8-5-3-2-4-7(8)10(6)13/h2-5H,1H3
InchiKey: WYIOQBYLZGEHCV-UHFFFAOYSA-N
Formula: C11H7ClO2
SMILES: CC1=C(Cl)C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 206.62
CAS: 17015-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-45.53	kJ/mol	Joback Method
hf	-214.63	kJ/mol	Joback Method
hfus	16.52	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	9.67 ± 0.05	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	2.578		Crippen Method
mcvol	142.310	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	680.61	K	Joback Method
tc	945.26	K	Joback Method
tf	463.49	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.16	J/mol×K	680.61	Joback Method
cpg	352.01	J/mol×K	724.72	Joback Method
cpg	363.89	J/mol×K	768.83	Joback Method
cpg	374.77	J/mol×K	812.94	Joback Method
cpg	384.62	J/mol×K	857.04	Joback Method
cpg	393.43	J/mol×K	901.15	Joback Method

cpg	401.18	J/mol×K	945.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17015995&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

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