1,4-Naphthalenedione, 2-hydroxy-3-methyl-

Other names:	1,4-Naphthoquinone, 2-hydroxy-3-methyl-
	Phthiocol
	Phthiokol
	2-Hydroxy-3-methyl-1,4-naphthoquinone
	2-Methyl-3-hydroxy-1,4-naphthoquinone
	3-Hydroxy-2-methyl-1,4-naphthoquinone
Inchi:	InChI=1S/C11H8O3/c1-6-9(12)7-4-2-3-5-8(7)11(14)10(6)13/h2-5,13H,1H3
InchiKey:	LULCPJWUGUVEFU-UHFFFAOYSA-N
Formula:	C11H8O3
SMILES:	CC1=C(O)C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	188.18
CAS:	483-55-6

Physical Properties

Property code	Value	Unit	Source
gf	-170.42	kJ/mol	Joback Method
hf	-351.12	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.898		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
tb	735.36	K	Joback Method
tc	973.28	K	Joback Method
tf	494.39	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.28	J/mol×K	735.36	Joback Method
cpg	373.32	J/mol×K	775.01	Joback Method
cpg	383.53	J/mol×K	814.67	Joback Method

cpg	392.88	J/mol×K	854.32	Joback Method
cpg	401.37	J/mol×K	893.97	Joback Method
cpg	408.97	J/mol×K	933.62	Joback Method
cpg	415.67	J/mol×K	973.28	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=C483556&Units=SI

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
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