1,4-Naphthalenedione, 2-(acetyloxy)-

Other names:	1,4-Naphthoquinone, 2-hydroxy-, acetate
	2-Acetoxy-1,4-naphthoquinone
	2-Hydroxy-1,4-naphthoquinone acetate
Inchi:	InChI=1S/C12H8O4/c1-7(13)16-11-6-10(14)8-4-2-3-5-9(8)12(11)15/h2-6H,1H3
InchiKey:	QHISPATYFAPAKC-UHFFFAOYSA-N
Formula:	C12H8O4
SMILES:	CC(=O)OC1=CC(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	216.19
CAS:	1785-65-5

Physical Properties

Property code	Value	Unit	Source
gf	-249.47	kJ/mol	Joback Method
hf	-452.86	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	64.24	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.513		Crippen Method
mcvol	151.600	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1833.00		NIST Webbook
tb	737.37	K	Joback Method
tc	993.32	K	Joback Method
tf	504.48	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.07	J/mol×K	737.37	Joback Method
cpg	415.91	J/mol×K	780.03	Joback Method
cpg	427.61	J/mol×K	822.69	Joback Method
cpg	438.12	J/mol×K	865.34	Joback Method
cpg	447.42	J/mol×K	908.00	Joback Method

cpg	455.46	J/mol×K	950.66	Joback Method
cpg	462.21	J/mol×K	993.32	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=C1785655&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume