1,4-Naphthalenedione, 2,3-dihydroxy-

Other names:	1,4-Naphthoquinone, 2,3-dihydroxy-
	Isonaphthazarin
	Isonaphthazarine
	2,3-Dihydroxy-1,4-naphthoquinone
	2,3-dihydroxy-1,4-naphthochinon
Inchi:	InChI=1S/C10H6O4/c11-7-5-3-1-2-4-6(5)8(12)10(14)9(7)13/h1-4,13-14H
InchiKey:	BVQUETZBXIMAFZ-UHFFFAOYSA-N
Formula:	C10H6O4
SMILES:	O=C1C(O)=C(O)C(=O)c2ccccc21
Mol. weight [g/mol]:	190.15
CAS:	605-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-315.66	kJ/mol	Joback Method
hf	-482.71	kJ/mol	Joback Method
hfus	17.91	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.393		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
rinpol	1241.00		NIST Webbook
tb	804.66	K	Joback Method
tc	1029.44	K	Joback Method
tf	543.94	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.58	J/mol×K	804.66	Joback Method
cpg	360.68	J/mol×K	842.12	Joback Method
cpg	368.06	J/mol×K	879.59	Joback Method

cpg	374.71	J/mol×K	917.05	Joback Method
cpg	380.61	J/mol×K	954.51	Joback Method
cpg	385.75	J/mol×K	991.97	Joback Method
cpg	390.11	J/mol×K	1029.44	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=C605378&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