1,4-Naphthalenedione, 5,8-dihydroxy-

Other names:	1,4-Naphthoquinone, 5,8-dihydroxy- Naphthazarin Naphthazarine Naphthazarone 5,8-Dihydroxy-1,4-naphthoquinone 5,8-Dihydroxynaphthoquinone 5,8-Dihydroxy-1,4-naphthalenedione 5,8-Dihydroxy-1,4-naphthosemiquinone NSC 26647
Inchi:	InChI=1S/C10H6O4/c11-5-1-2-6(12)10-8(14)4-3-7(13)9(5)10/h1-4,11-12H
InchiKey:	RQNVIKXOOKXAJQ-UHFFFAOYSA-N
Formula:	C10H6O4
SMILES:	O=C1C=CC(=O)c2c(O)ccc(O)c21
Mol. weight [g/mol]:	190.15
CAS:	475-38-7

Physical Properties

Property code	Value	Unit	Source
chs	-4196.80 ± 0.50	kJ/mol	NIST Webbook
gf	-332.00	kJ/mol	Joback Method
hf	-499.10 ± 3.20	kJ/mol	NIST Webbook
hfs	-595.80 ± 2.10	kJ/mol	NIST Webbook
hfus	22.08	kJ/mol	Joback Method
hsub	96.70	kJ/mol	NIST Webbook
hvap	76.00	kJ/mol	Joback Method
ie	8.20 ± 0.02	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.033		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
tb	771.58	K	Joback Method
tc	1051.15	K	Joback Method
tf	620.70	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.03	J/mol×K	771.58	Joback Method
cpg	363.33	J/mol×K	818.17	Joback Method
cpg	373.15	J/mol×K	864.77	Joback Method
cpg	382.64	J/mol×K	911.36	Joback Method
cpg	391.95	J/mol×K	957.96	Joback Method
cpg	401.24	J/mol×K	1004.55	Joback Method
cpg	410.65	J/mol×K	1051.15	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C475387&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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