1,4-Naphthalenedione, 2,5,8-trihydroxy-

Other names: 1,4-Naphthoquinone, 2,5,8-trihydroxy-
Naphthopurpurin
Inchi: InChI=1S/C10H6O5/c11-4-1-2-5(12)9-8(4)6(13)3-7(14)10(9)15/h1-3,11-12,14H
InchiKey: ZFXYVCPRQYVJDR-UHFFFAOYSA-N
Formula: C10H6O5
SMILES: O=C1C=C(O)C(=O)c2c(O)ccc(O)c21
Mol. weight [g/mol]: 206.15
CAS: 13379-22-1

Physical Properties

Property code	Value	Unit	Source
gf	-478.45	kJ/mol	Joback Method
hf	-673.63	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	0.919		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	7026.18	kPa	Joback Method
tb	868.74	K	Joback Method
tc	1122.77	K	Joback Method
tf	694.04	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.16	J/mol×K	868.74	Joback Method
cpg	397.93	J/mol×K	911.08	Joback Method
cpg	406.55	J/mol×K	953.42	Joback Method
cpg	415.10	J/mol×K	995.75	Joback Method
cpg	423.71	J/mol×K	1038.09	Joback Method
cpg	432.47	J/mol×K	1080.43	Joback Method
cpg	441.49	J/mol×K	1122.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13379221&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
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