1,2-Naphthalenedione

Other names: «beta»-Naphthoquinone
o-Naphthoquinone
1,2-Naphthoquinone
Naphthoquinone-(1,2)
1,2-Naphthaquinone
1,2-Naftochinon
Inchi: InChI=1S/C10H6O2/c11-9-6-5-7-3-1-2-4-8(7)10(9)12/h1-6H
InchiKey: KETQAJRQOHHATG-UHFFFAOYSA-N
Formula: C10H6O2
SMILES: O=C1C=Cc2ccccc2C1=O
Mol. weight [g/mol]: 158.15
CAS: 524-42-5

Physical Properties

Property code	Value	Unit	Source
chs	-4629.20	kJ/mol	NIST Webbook
gf	-22.76	kJ/mol	Joback Method
hf	-155.31	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	49.97	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.465		Crippen Method
mcvol	115.980	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	264.10		NIST Webbook
tb	610.34	K	Joback Method
tc	877.21	K	Joback Method
tf	397.26	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.12	J/mol×K	610.34	Joback Method

cpg	284.57	J/mol×K	654.82	Joback Method
cpg	297.05	J/mol×K	699.30	Joback Method
cpg	308.56	J/mol×K	743.78	Joback Method
cpg	319.09	J/mol×K	788.26	Joback Method
cpg	328.63	J/mol×K	832.73	Joback Method
cpg	337.17	J/mol×K	877.21	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=C524425&Units=SI

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
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

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