1,2-Naphthoquinone

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]:	158.16

Physical Properties

Property code	Value	Unit	Source
chs	-4629.20	kJ/mol	NIST Webbook
hf	-61.95	kJ/mol	Cheméo Relay (1.0)
hfus	10.51	kJ/mol	Joback Method
ie	8.72	eV	Cheméo Relay (1.0)
log10ws	-2.50		Cheméo Relay (1.0)
logp	1.465		Crippen Method
mcvol	115.980	ml/mol	McGowan Method
rinpol	264.10		NIST Webbook
tb	558.35	K	Cheméo Relay (1.0)
tf	398.12	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C524425&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point