1,4-Naphthalenedione

Other names:	.alpha.-naphthoquinone
	1,4-Dihydro-1,4-diketonaphthalene
	1,4-Naftochinon
	1,4-Naphthoquinone
	1,4-Naphthylquinone
	1,4-naphthaquinone
	NSC 9583
	Naphthoquinone
	Rcra waste number U166
	USAF CY-10
	p-Naphthoquinone
	«alpha»-Naphthoquinone
Inchi:	InChI=1S/C10H6O2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H
InchiKey:	FRASJONUBLZVQX-UHFFFAOYSA-N
Formula:	C10H6O2
SMILES:	O=C1C=CC(=O)c2ccccc21
Mol. weight [g/mol]:	158.15
CAS:	130-15-4

Physical Properties

Property code	Value	Unit	Source
chs	-4604.10 ± 1.10	kJ/mol	NIST Webbook
chs	-4605.70	kJ/mol	NIST Webbook
chs	-4608.92	kJ/mol	NIST Webbook
ea	1.81 ± 0.11	eV	NIST Webbook
ea	1.80 ± 0.05	eV	NIST Webbook
ea	0.80	eV	NIST Webbook
ea	0.60	eV	NIST Webbook
gf	-22.76	kJ/mol	Joback Method
hf	-97.50 ± 1.90	kJ/mol	NIST Webbook
hfs	-188.50 ± 1.70	kJ/mol	NIST Webbook
hfus	10.51	kJ/mol	Joback Method
hsub	91.00 ± 0.80	kJ/mol	NIST Webbook
hsub	72.40	kJ/mol	NIST Webbook
hsub	91.00 ± 0.80	kJ/mol	NIST Webbook
hsub	91.00	kJ/mol	NIST Webbook
hvap	49.97	kJ/mol	Joback Method

ie	9.67 ± 0.02	eV	NIST Webbook
ie	9.56 ± 0.01	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.49	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	1.622		Crippen Method
mcvol	115.980	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	241.60		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	241.61		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	241.61		NIST Webbook
rinpol	241.61		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	240.82		NIST Webbook
rinpol	240.82		NIST Webbook
rinpol	1418.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2205.00		NIST Webbook
tb	610.34	K	Joback Method
tc	877.21	K	Joback Method
tf	399.15 ± 2.00	K	NIST Webbook
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.63	J/mol×K	832.73	Joback Method
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	337.17	J/mol×K	877.21	Joback Method
hsubt	91.00 ± 2.00	kJ/mol	313.00	NIST Webbook

Sources

Measurement and Correlation of 1,4-Naphthoquinone and of Plumbagin Solubilities in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je200675g
Solubilities of 1,4-Naphthoquinone in Acetone, Toluene, Xylene, Ethanol, and n-Butyl Alcohol:	https://www.doi.org/10.1021/je800405b
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=C130154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume