1,4-NAPHTHALENEDIOL

Other names:	1,4-Dihydroxynaphthalene
	1,4-Naphthohydroquinone
	1,4-Naphththalenediol
	Hydronaphthoquinone
	Naphthalenediol-(1,4)
	Naphthohydroquinone
	naphthalene-1,4-diol
Inchi:	InChI=1S/C10H8O2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6,11-12H
InchiKey:	PCILLCXFKWDRMK-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	Oc1ccc(O)c2ccccc12
Mol. weight [g/mol]:	160.17

Physical Properties

Property code	Value	Unit	Source
af	0.6470		Cheméo Relay (1.0)
chs	-4739.00 ± 7.00	kJ/mol	NIST Webbook
chs	-4761.00 ± 0.70	kJ/mol	NIST Webbook
chs	-4770.00 ± 30.00	kJ/mol	NIST Webbook
gf	-56.86	kJ/mol	Joback Method
hf	-197.00 ± 1.80	kJ/mol	NIST Webbook
hfs	-317.40 ± 1.50	kJ/mol	NIST Webbook
hfus	24.28	kJ/mol	Joback Method
hsub	120.40	kJ/mol	NIST Webbook
hsub	120.40 ± 1.00	kJ/mol	NIST Webbook
hsub	150.00 ± 8.00	kJ/mol	NIST Webbook
hvap	97.47	kJ/mol	Cheméo Relay (1.0)
ie	7.62 ± 0.03	eV	NIST Webbook
log10ws	-2.52		Cheméo Relay (1.0)
logp	2.251		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
pc	5880.91	kPa	Joback Method
tb	570.16	K	Cheméo Relay (1.0)
tc	878.29	K	Cheméo Relay (1.0)
tf	460.24	K	Cheméo Relay (1.0)
vc	0.417	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.88	J/mol×K	852.16	Joback Method
cpg	349.82	J/mol×K	895.57	Joback Method
cpg	308.81	J/mol×K	678.51	Joback Method
cpg	317.75	J/mol×K	721.92	Joback Method
cpg	326.08	J/mol×K	765.34	Joback Method
cpg	334.05	J/mol×K	808.75	Joback Method
cpg	299.04	J/mol×K	635.10	Joback Method
dvisc	0.0000420	Pa×s	535.05	Joback Method
dvisc	0.0000728	Pa×s	510.03	Joback Method
dvisc	0.0001338	Pa×s	485.02	Joback Method
dvisc	0.0000254	Pa×s	560.06	Joback Method
dvisc	0.0000161	Pa×s	585.07	Joback Method
dvisc	0.0000105	Pa×s	610.09	Joback Method
dvisc	0.0000071	Pa×s	635.10	Joback Method
hsubt	119.00 ± 1.00	kJ/mol	381.00	NIST Webbook

Sources

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=C571608&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume