1-Naphthalenol

Other names:	.alpha.-naphthol
	1-Hydroxynaphthalene
	1-Naphthol
	1-Napthol
	Basf Ursol ERN
	C.I. 76605
	C.I. Oxidation Base 33
	Durafur Developer D
	Fouramine ERN
	Fourrine 99
	Fourrine ERN
	Furro ER
	NSC 9586
	Nako TRB
	Tertral ERN
	Ursol ERN
	Zoba ERN
	«alpha»-Hydroxynaphthalene
	«alpha»-Naphthol
	Â«alphaÂ»-Hydroxynaphthalene
	Â«alphaÂ»-Naphthol
Inchi:	InChI=1S/C10H8O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7,11H
InchiKey:	KJCVRFUGPWSIIH-UHFFFAOYSA-N
Formula:	C10H8O
SMILES:	Oc1cccc2ccccc12
Mol. weight [g/mol]:	144.17
CAS:	90-15-3

Physical Properties

Property code	Value	Unit	Source
chs	-4956.40 ± 0.80	kJ/mol	NIST Webbook
chs	-4959.70	kJ/mol	NIST Webbook
chs	-4951.10 ± 4.90	kJ/mol	NIST Webbook
chs	-4965.60 ± 2.10	kJ/mol	NIST Webbook
chs	-4957.33 ± 0.88	kJ/mol	NIST Webbook
chs	-4983.00	kJ/mol	NIST Webbook

gf	97.76	kJ/mol	Joback Method
hf	-30.80 ± 1.60	kJ/mol	NIST Webbook
hf	-29.90 ± 1.10	kJ/mol	NIST Webbook
hf	-4.30	kJ/mol	NIST Webbook
hfs	-95.40	kJ/mol	NIST Webbook
hfs	-121.00 ± 1.00	kJ/mol	NIST Webbook
hfs	-122.00 ± 1.50	kJ/mol	NIST Webbook
hfus	18.50	kJ/mol	Joback Method
hsub	91.50 ± 3.80	kJ/mol	NIST Webbook
hsub	91.20	kJ/mol	NIST Webbook
hsub	91.17 ± 0.42	kJ/mol	NIST Webbook
hsub	91.10	kJ/mol	NIST Webbook
hvap	54.78	kJ/mol	Joback Method
ie	7.76 ± 0.03	eV	NIST Webbook
ie	7.78	eV	NIST Webbook
ie	7.76 ± 0.03	eV	NIST Webbook
log10ws	-2.22		Estimated Solubility Method
log10ws	-2.08		Aqueous Solubility Prediction Method
logp	2.545		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
rinpol	258.48		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	258.80		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	258.50		NIST Webbook
rinpol	259.66		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	259.66		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1494.90		NIST Webbook
rinpol	1473.70		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1517.00		NIST Webbook

rinpol	1494.00		NIST Webbook
rinpol	1464.00		NIST Webbook
tb	553.15	K	NIST Webbook
tb	552.20	K	NIST Webbook
tb	561.16 ± 0.15	K	NIST Webbook
tc	805.35	K	Joback Method
tf	368.65	K	Aqueous Solubility Prediction Method
tf	370.54	K	Thermodynamic Data for Processing Naphthol with Supercritical Carbon Dioxide
tt	368.20 ± 0.30	K	NIST Webbook
tt	368.49	K	Thermodynamic properties of 1-naphthol: Mutual validation of experimental and computational results
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.55	J/mol×K	721.72	Joback Method
cpg	306.83	J/mol×K	763.54	Joback Method
cpg	257.18	J/mol×K	554.48	Joback Method
cpg	269.06	J/mol×K	596.29	Joback Method
cpg	279.81	J/mol×K	638.10	Joback Method
cpg	289.59	J/mol×K	679.91	Joback Method
cpg	314.59	J/mol×K	805.35	Joback Method
cps	285.00	J/mol×K	393.00	NIST Webbook
cps	166.90	J/mol×K	298.00	NIST Webbook
dvisc	0.0001179	Pa×s	524.28	Joback Method
dvisc	0.0000819	Pa×s	554.48	Joback Method
dvisc	0.0017549	Pa×s	373.30	Joback Method
dvisc	0.0008699	Pa×s	403.50	Joback Method
dvisc	0.0004755	Pa×s	433.69	Joback Method
dvisc	0.0002811	Pa×s	463.89	Joback Method
dvisc	0.0001773	Pa×s	494.09	Joback Method
hfust	23.47	kJ/mol	368.20	NIST Webbook
hfust	23.47	kJ/mol	368.20	NIST Webbook
hfust	23.30	kJ/mol	368.70	NIST Webbook
hfust	24.40	kJ/mol	369.70	NIST Webbook
hfust	23.01	kJ/mol	369.00	NIST Webbook

hfust	23.22	kJ/mol	369.00	NIST Webbook
hsubt	91.20 ± 0.40	kJ/mol	304.50	NIST Webbook
hsubt	71.50	kJ/mol	561.01	NIST Webbook
hsubt	93.30	kJ/mol	305.00	NIST Webbook
hsubt	84.30	kJ/mol	319.00	NIST Webbook
hsubt	89.10 ± 1.70	kJ/mol	303.50	NIST Webbook
hvapt	60.80	kJ/mol	493.00	NIST Webbook
hvapt	58.50	kJ/mol	477.50	NIST Webbook
sfust	63.60	J/mol×K	368.20	NIST Webbook
sfust	62.90	J/mol×K	369.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39840e+01
Coeff. B	-4.01524e+03
Coeff. C	-1.23482e+02
Temperature range (K), min.	410.35
Temperature range (K), max.	586.46

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermodynamic properties of 1-naphthol: Mutual validation of experimental and computational results:	https://www.doi.org/10.1016/j.jct.2015.02.008
Densities and Viscosities of Naphthalen-1-ol, Naphthalen-2-ol, and 1-Aminonaphthalene in the Solvents of Ethanol, Propan-1-ol, and Butan-1-ol:	https://www.doi.org/10.1021/je201222n
Thermodynamic Data for Processing Naphthol with Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.6b00781
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume