2-Naphthalenol

Other names:

.beta.-hydroxynaphthalene
.beta.-naphthol
2-Hydroxynaphthalene
2-Naftol
2-Naftolo
2-Naphthol
2-Naphtol
2-Napthol
Antioxygene BN
Azogen Developer A
Betanaphthol
C.I. 37500
C.I. Azoic Coupling Component 1
C.I. Developer 5
Developer A
Developer AMS
Developer BN
Isonaphthol
NSC 2044
Naphthol B
Naphthol, «beta»
Naphthol, Â«betaÂ»
«beta»-Hydroxynaphthalene
«beta»-Monoxynaphthalene
«beta»-Naftol
«beta»-Naftolo
«beta»-Naphthol
«beta»-Naphthyl alcohol
«beta»-Naphthyl hydroxide
«beta»-Naphtol
«beta»-Napthol
Â«betaÂ»-Hydroxynaphthalene
Â«betaÂ»-Monoxynaphthalene
Â«betaÂ»-Naftol
Â«betaÂ»-Naftolo
Â«betaÂ»-Naphthol
Â«betaÂ»-Naphthyl alcohol
Â«betaÂ»-Naphthyl hydroxide
Â«betaÂ»-Naphtol
Â«betaÂ»-Napthol

Inchi: InChI=1S/C10H8O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7,11H
InchiKey: JWAZRIHNYRIHIV-UHFFFAOYSA-N
Formula: C10H8O
SMILES: Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 144.17
CAS: 135-19-3

Physical Properties

Property code	Value	Unit	Source
gf	97.76	kJ/mol	Joback Method
hf	-29.90 ± 1.70	kJ/mol	NIST Webbook
hf	-13.80	kJ/mol	NIST Webbook
hf	-30.00 ± 1.10	kJ/mol	NIST Webbook
hfs	-124.10 ± 1.60	kJ/mol	NIST Webbook
hfs	-124.20 ± 1.00	kJ/mol	NIST Webbook
hfs	-108.00	kJ/mol	NIST Webbook
hfus	21.07	kJ/mol	Phase Equilibria, Crystallization, and Microstructural Studies of Naphthalen-2-ol + 1,3-Dinitrobenzene
hsub	83.00 ± 3.80	kJ/mol	NIST Webbook
hsub	94.18 ± 0.50	kJ/mol	NIST Webbook
hsub	85.50 ± 1.20	kJ/mol	NIST Webbook
hsub	78.70 ± 0.80	kJ/mol	NIST Webbook
hsub	94.20	kJ/mol	NIST Webbook
hsub	94.20	kJ/mol	NIST Webbook
hvap	76.20	kJ/mol	NIST Webbook
ie	7.87 ± 0.02	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
ie	7.85 ± 0.05	eV	NIST Webbook
ie	7.89 ± 0.06	eV	NIST Webbook
log10ws	-2.16		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.28		Estimated Solubility Method
log10ws	-2.27		Aqueous Solubility Prediction Method
logp	2.545		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
rinpol	1522.00		NIST Webbook

rinpol	260.22		NIST Webbook
rinpol	1520.50		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1520.10		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1531.00		NIST Webbook
rinpol	1520.50		NIST Webbook
rinpol	1520.10		NIST Webbook
rinpol	1514.50		NIST Webbook
rinpol	1520.50		NIST Webbook
rinpol	1523.80		NIST Webbook
rinpol	1560.10		NIST Webbook
rinpol	1514.50		NIST Webbook
rinpol	1520.50		NIST Webbook
rinpol	1523.80		NIST Webbook
rinpol	1520.50		NIST Webbook
rinpol	1520.10		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	260.22		NIST Webbook
rinpol	259.70		NIST Webbook
rinpol	260.22		NIST Webbook
rinpol	1560.10		NIST Webbook
sg	366.60 ± 3.90	J/mol×K	NIST Webbook
ss	179.00	J/mol×K	NIST Webbook
tb	558.70	K	NIST Webbook
tb	568.00 ± 0.30	K	NIST Webbook
tb	559.00 ± 0.40	K	NIST Webbook
tc	805.35	K	Joback Method
tf	394.00 ± 1.00	K	NIST Webbook
tf	396.98	K	Thermodynamic Data for Processing Naphthol with Supercritical Carbon Dioxide
tf	394.35 ± 0.10	K	Phase Equilibria, Crystallization, and Microstructural Studies of Naphthalen-2-ol + 1,3-Dinitrobenzene
tf	395.15 ± 2.00	K	NIST Webbook
tf	395.55	K	Aqueous Solubility Prediction Method

tf	396.15 ± 1.00	K	NIST Webbook
tf	394.55 ± 0.20	K	NIST Webbook
tf	394.65 ± 0.15	K	NIST Webbook
tf	390.00 ± 1.50	K	NIST Webbook
tf	393.00 ± 3.00	K	NIST Webbook
tf	395.25 ± 0.20	K	NIST Webbook
tf	394.00 ± 0.30	K	NIST Webbook
tt	393.80 ± 1.25	K	NIST Webbook
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.59	J/mol×K	805.35	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	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
cps	172.80	J/mol×K	298.00	NIST Webbook
dvisc	0.0001179	Pa×s	524.28	Joback Method
dvisc	0.0001773	Pa×s	494.09	Joback Method
dvisc	0.0002811	Pa×s	463.89	Joback Method
dvisc	0.0004755	Pa×s	433.69	Joback Method
dvisc	0.0008699	Pa×s	403.50	Joback Method
dvisc	0.0000819	Pa×s	554.48	Joback Method
dvisc	0.0017549	Pa×s	373.30	Joback Method
hfust	20.90	kJ/mol	388.00	NIST Webbook
hfust	18.79	kJ/mol	393.60	NIST Webbook
hfust	18.79	kJ/mol	393.60	NIST Webbook
hsubt	87.80	kJ/mol	323.00	NIST Webbook
hsubt	97.80	kJ/mol	305.00	NIST Webbook
hsubt	94.20 ± 0.50	kJ/mol	314.00	NIST Webbook
hsubt	87.40 ± 2.50	kJ/mol	300.50	NIST Webbook
hsubt	68.20	kJ/mol	567.85	NIST Webbook
hsubt	78.66 ± 0.84	kJ/mol	283.00	NIST Webbook
hvapt	61.80	kJ/mol	493.00	NIST Webbook
hvapt	59.70	kJ/mol	489.00	NIST Webbook
hvapt	59.70	kJ/mol	481.00	NIST Webbook
sfust	55.90	J/mol×K	393.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Phase Equilibria, Crystallization, and Microstructural Studies of Naphthalen-2-ol + 1,3-Dinitrobenzene:	https://www.doi.org/10.1021/je100358e
Thermodynamic Data for Processing Naphthol with Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/acs.jced.6b00781
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135193&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume