8-Hydroxyquinoline

Other names:	1-Azanaphthalene-8-ol
	8-Chinolinol
	8-Hydroxychinolin
	8-OQ
	8-Oxyquinolin
	8-Oxyquinoline
	8-Quinol
	8-Quinolinol
	8-Quinolol
	Bioquin
	Fennosan
	Fennosan H 30
	Hydroxybenzopyridine
	NCI-C55298
	NSC 2039
	NSC 615011
	NSC 82404
	Oxin
	Oxine
	Oxoquinoline
	Oxybenzopyridine
	Oxychinolin
	Oxychinoline
	Oxyquinoline
	Phenopyridine
	Quinolin-8-ol
	Quinophenol
	Tumex
	USAF EK-794
	o-Oxychinolin
	quinoline, 8-hydroxy-
Inchi:	InChI=1S/C9H7NO/c11-8-5-1-3-7-4-2-6-10-9(7)8/h1-6,11H
InchiKey:	MCJGNVYPOGVAJF-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	Oc1cccc2cccnc12
Mol. weight [g/mol]:	145.16
CAS:	148-24-3

Physical Properties

Property code	Value	Unit	Source
chs	-4459.00 ± 0.90	kJ/mol	NIST Webbook
chs	-4457.20 ± 8.40	kJ/mol	NIST Webbook
chs	-4455.50 ± 0.80	kJ/mol	NIST Webbook
chs	-4467.70	kJ/mol	NIST Webbook
chs	-4460.80 ± 1.60	kJ/mol	NIST Webbook
hf	6.50 ± 1.70	kJ/mol	NIST Webbook
hf	27.60 ± 2.60	kJ/mol	NIST Webbook
hfs	-81.20 ± 2.00	kJ/mol	NIST Webbook
hfs	-83.00 ± 1.50	kJ/mol	NIST Webbook
hsub	87.90 ± 0.80	kJ/mol	NIST Webbook
hsub	109.00 ± 0.80	kJ/mol	NIST Webbook
hsub	108.80 ± 1.70	kJ/mol	NIST Webbook
hsub	89.00 ± 1.40	kJ/mol	NIST Webbook
hsub	89.50 ± 0.90	kJ/mol	NIST Webbook
hsub	89.50 ± 0.90	kJ/mol	NIST Webbook
log10ws	-2.42		Aqueous Solubility Prediction Method
log10ws	-2.42		Estimated Solubility Method
logp	1.940		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
rinpol	232.24		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1326.30		NIST Webbook
rinpol	1348.90		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1339.00		NIST Webbook
ripol	2153.00		NIST Webbook
tf	347.65 ± 2.00	K	NIST Webbook
tf	348.32	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	40.30	kJ/mol	345.70	NIST Webbook

hfust	22.10	kJ/mol	346.80	NIST Webbook
hsubt	108.80 ± 1.70	kJ/mol	318.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	540.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.01590e+02
Coeff. B	-1.21996e+04
Coeff. C	-1.19913e+01
Coeff. D	3.59759e-06
Temperature range (K), min.	346.00
Temperature range (K), max.	788.00

Sources

Synthesis, Characterization and Standard Molar Enthalpy of Formation of Sm(C7H5O3)2·(C9H6NO):	https://www.doi.org/10.1016/j.tca.2007.10.003
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1364
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Synthesis, characterization and standard molar enthalpy of formation of La(C7H5O3)2(C9H6NO):	https://www.doi.org/10.1016/j.tca.2005.10.015
Thermochemical Approach on Rare Earth Complex of Gadolinium with Salicylic acid and 8-hydroxyquinoline:	https://www.doi.org/10.1016/j.tca.2012.08.027
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1364.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148243&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point