1(2H)-ISOQUINOLINONE

Other names:	1(2H)-Isoquinolone
	1-hydroxyisoquinoline
	1-isoquinolinol
	Isocarbostyril
	Isoquinolin-1-one
Inchi:	InChI=1S/C9H7NO/c11-9-8-4-2-1-3-7(8)5-6-10-9/h1-6H,(H,10,11)
InchiKey:	VDBNYAPERZTOOF-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	O=c1[nH]ccc2ccccc12
Mol. weight [g/mol]:	145.16

Physical Properties

Property code	Value	Unit	Source
hf	-6.32	kJ/mol	Cheméo Relay (1.0)
hsub	113.60 ± 2.20	kJ/mol	NIST Webbook
hvap	88.22	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	1.046		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
pc	4788.01	kPa	Cheméo Relay (1.0, beta)
tb	586.39	K	Cheméo Relay (1.0)
tc	857.94	K	Cheméo Relay (1.0)
tf	424.35	K	Cheméo Relay (1.0)
vc	0.401	m3/kmol	Cheméo Relay (1.0)

Sources

Thermochemical studies of 1-hydroxyisoquinoline, 8-hydroxyisoquinoline and 1,5-dihydroxyisoquinoline:	https://www.doi.org/10.1016/j.jct.2005.03.009
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C491305&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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