

7-QUINOLINOL

Other names:	7-Hydroxyquinoline quinolin-7-ol
Inchi:	InChI=1S/C9H7NO/c11-8-4-3-7-2-1-5-10-9(7)6-8/h1-6,11H
InchiKey:	XCRPPAPDRUBKRJ-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	Oc1ccc2cccnc2c1
Mol. weight [g/mol]:	145.16

Physical Properties

Property code	Value	Unit	Source
af	0.5530		Cheméo Relay (1.0)
hf	21.00	kJ/mol	Cheméo Relay (1.0)
hvap	83.68	kJ/mol	Cheméo Relay (1.0)
ie	8.37	eV	Cheméo Relay (1.0)
log10ws	-1.48		Cheméo Relay (1.0)
logp	1.940		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
pc	5846.25	kPa	Cheméo Relay (1.0, beta)
tb	579.01	K	Cheméo Relay (1.0)
tc	870.97	K	Cheméo Relay (1.0)
tf	511.00 ± 3.00	K	NIST Webbook
vc	0.396	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C580201&Units=SI>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
hf:	Enthalpy of formation 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

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