3-CYANOINDOLE

Other names:	3-Cyanoindole
	Indole-3-carbonitrile
Inchi:	InChI=1S/C9H6N2/c10-5-7-6-11-9-4-2-1-3-8(7)9/h1-4,6,11H
InchiKey:	CHIFTAQVXHNVRW-UHFFFAOYSA-N
Formula:	C9H6N2
SMILES:	N#Cc1c[nH]c2ccccc12
Mol. weight [g/mol]:	142.16

Physical Properties

Property code	Value	Unit	Source
hf	295.84	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
log10ws	-2.79		Cheméo Relay (1.0)
logp	1.558		Crippen Method
mcvol	110.110	ml/mol	McGowan Method
tb	594.08	K	Cheméo Relay (1.0)
tf	413.85	K	Cheméo Relay (1.0)

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5457283&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point