5H-1-Pyrindine, 6,7-dihydro-

Other names:	2,3-Cyclopentenopyridine
	Pyrindan
	Cyclopenta[b]pyridine
	5H-1-Pyrindene, 6,7-dihydro-
	6,7-dihydro-5H-cyclopenta(b)pyridine
Inchi:	InChI=1S/C8H9N/c1-3-7-4-2-6-9-8(7)5-1/h2,4,6H,1,3,5H2
InchiKey:	KRNSYSYRLQDHDK-UHFFFAOYSA-N
Formula:	C8H9N
SMILES:	c1cnc2c(c1)CCC2
Mol. weight [g/mol]:	119.16
CAS:	533-37-9

Physical Properties

Property code	Value	Unit	Source
affp	957.50	kJ/mol	NIST Webbook
basg	925.60	kJ/mol	NIST Webbook
ie	9.15	eV	NIST Webbook
log10ws	-2.32		Crippen Method
logp	1.570		Crippen Method
mcvol	98.940	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.70	K	1.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C533379&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure