1H-Indole, 7-methyl-

Other names: Indole, 7-methyl-
7-Methylindol
7-Methylindole
Inchi: InChI=1S/C9H9N/c1-7-3-2-4-8-5-6-10-9(7)8/h2-6,10H,1H3
InchiKey: KGWPHCDTOLQQEP-UHFFFAOYSA-N
Formula: C9H9N
SMILES: Cc1cccc2cc[nH]c12
Mol. weight [g/mol]: 131.17
CAS: 933-67-5

Physical Properties

Property code	Value	Unit	Source
ie	7.71 ± 0.00	eV	NIST Webbook
ie	7.71 ± 0.00	eV	NIST Webbook
ie	7.53 ± 0.01	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	1.994		Crippen Method
mcvol	108.730	ml/mol	McGowan Method
rinpol	1383.20		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1383.20		NIST Webbook
rinpol	235.49		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2430.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	539.20	K	NIST Webbook
tf	356.00 ± 2.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C933675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point