1H-Indole, 5-methyl-

Other names: Indole, 5-methyl-
5-Methylindol
5-Methylindole
Inchi: InChI=1S/C9H9N/c1-7-2-3-9-8(6-7)4-5-10-9/h2-6,10H,1H3
InchiKey: YPKBCLZFIYBSHK-UHFFFAOYSA-N
Formula: C9H9N
SMILES: Cc1ccc2[nH]ccc2c1
Mol. weight [g/mol]: 131.17
CAS: 614-96-0

Physical Properties

Property code	Value	Unit	Source
ie	7.38 ± 0.00	eV	NIST Webbook
log10ws	-2.97		Crippen Method
logp	1.994		Crippen Method
mcvol	108.730	ml/mol	McGowan Method
rinpol	1392.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1391.00		NIST Webbook
ripol	2468.00		NIST Webbook
ripol	2461.00		NIST Webbook
ripol	2468.00		NIST Webbook
ripol	2461.00		NIST Webbook
ripol	2493.00		NIST Webbook
tb	540.20	K	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C614960&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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