

5-Aminoindazole

Other names:	1H-Indazol-5-amine 1H-Indazole, 5-amino- 5-Amino-1H-indazole indazol-5-ylamine
Inchi:	InChI=1S/C7H7N3/c8-6-1-2-7-5(3-6)4-9-10-7/h1-4H,8H2,(H,9,10)
InchiKey:	XBTOSRUBOXQWBO-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	<chem>Nc1ccc2[nH]ncc2c1</chem>
Mol. weight [g/mol]:	133.15
CAS:	19335-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Crippen Method
logp	0.663		Crippen Method
mcpvol	100.510	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhos	1400.00	kg/m3	295.10	Experimental and computational study of the energetics of 5- and 6-aminoindazole

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational study of the energetics of 5- and 6-aminoindazole:	https://www.doi.org/10.1016/j.jct.2010.04.026
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19335116&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density

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