

1H-Indole, 5-bromo-

Other names:	5-Bromoindole
Inchi:	InChI=1S/C8H6BrN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-5,10H
InchiKey:	VXWVFZFYXOBTA-UHFFFAOYSA-N
Formula:	C8H6BrN
SMILES:	Brc1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	196.04
CAS:	10075-50-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.66		Crippen Method
logp	2.449		Crippen Method
mcvol	112.140	ml/mol	McGowan Method

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=C10075500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/88-248-0/1H-Indole-5-bromo.pdf>

Generated by Cheméo on 2024-04-20 07:45:42.744659217 +0000 UTC m=+15888391.665236532.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.