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: VXWVFZFZYXOBTA-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/ci990307l

Legend

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