

Benzimidazoline,2-isopropylidene-1,3-dimethyl-

Inchi: InChI=1S/C12H16N2/c1-9(2)12-13(3)10-7-5-6-8-11(10)14(12)4/h5-8H,1-4H3
InchiKey: QJFVNVGUTOLOA-UHFFFAOYSA-N
Formula: C12H16N2
SMILES: CC(C)=C1N(C)c2ccccc2N1C
Mol. weight [g/mol]: 188.27
CAS: 143268-49-9

Physical Properties

Property code	Value	Unit	Source
ie	6.33	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.824		Crippen Method
mcvol	160.980	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C143268499&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

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<https://www.chemeo.com/cid/25-861-8/Benzimidazoline-2-isopropylidene-1-3-dimethyl.pdf>

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