

Benzoxazoline,2-isopropylidene-3-methyl-

Inchi:	InChI=1S/C11H13NO/c1-8(2)11-12(3)9-6-4-5-7-10(9)13-11/h4-7H,1-3H3
InchiKey:	SCKWCGDUCJVVHY-UHFFFAOYSA-N
Formula:	C11H13NO
SMILES:	CC(C)=C1Oc2ccccc2N1C
Mol. weight [g/mol]:	175.23
CAS:	143268-59-1

Physical Properties

Property code	Value	Unit	Source
ie	6.85	eV	NIST Webbook
log10ws	-3.08		Crippen Method
logp	2.767		Crippen Method
mcvol	142.780	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C143268591&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/86-137-5/Benzoxazoline-2-isopropylidene-3-methyl.pdf>

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