

4,5-Dimethyl-2-isobutyloxazole

Other names:	Oxazole, 4,5-dimethyl-2-(2-methylpropyl)- 2-iso-Butyl-4,5-dimethyloxazole 2-Isobutyl-4,5-dimethyl-1,3-oxazole Oxazole, 4,5-dimethyl-2-isobutyl 4,5-Dimethyl-2-(2-methylpropyl)-1,3-oxazole
Inchi:	InChI=1S/C9H15NO/c1-6(2)5-9-10-7(3)8(4)11-9/h6H,5H2,1-4H3
InchiKey:	SNRVAFQIIFPYDR-UHFFFAOYSA-N
Formula:	C9H15NO
SMILES:	<chem>Cc1nc(CC(C)C)oc1C</chem>
Mol. weight [g/mol]:	153.22
CAS:	26131-91-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.32		Crippen Method
logp	2.490		Crippen Method
mcvol	134.060	ml/mol	McGowan Method
rinpol	1044.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1330.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26131919&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

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/14-192-3/4-5-Dimethyl-2-isobutyloxazole.pdf>

Generated by Cheméo on 2024-04-27 09:32:00.296117239 +0000 UTC m=+16499569.216694555.

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