

2-isopropyl-4(5)-methyloxazole

Inchi: InChI=1S/C7H11NO/c1-5(2)7-8-6(3)4-9-7/h4-5H,1-3H3
InchiKey: HINVVVUEAOKCCA-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: Cc1coc(C(C)C)n1
Mol. weight [g/mol]: 125.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.63		Crippen Method
logp	2.106		Crippen Method
mcvol	105.880	ml/mol	McGowan Method
ripol	1203.00		NIST Webbook
ripol	1203.00		NIST Webbook
ripol	1203.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R296801&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/92-717-4/2-isopropyl-4-5-methyloxazole.pdf>

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