Oxazole, 5-methyl

Inchi: InChI=1S/C4H5NO/c1-4-2-5-3-6-4/h2-3H,1H3
InchiKey: ZYMHCFYHVYGFMS-UHFFFAOYSA-N
Formula: C4H5NO
SMILES: Cc1cnco1
Mol. weight [g/mol]: 83.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	0.983		Crippen Method
mcvol	63.610	ml/mol	McGowan Method
rinpol	683.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	683.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1102.00		NIST Webbook
ripol	1102.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R46217&Units=SI

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