Oxazole, 5-ethyl-4-methyl

Inchi: InChI=1S/C6H9NO/c1-3-6-5(2)7-4-8-6/h4H,3H2,1-2H3
InchiKey: ZLLASJMIAQWDJH-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: CCc1ocnc1C
Mol. weight [g/mol]: 111.14
CAS: 29584-92-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.25		Crippen Method
logp	1.545		Crippen Method
mcvol	91.790	ml/mol	McGowan Method
rinpol	851.00		NIST Webbook
ripol	1204.00		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=C29584927&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

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