Ethyl isoxazole-5-carboxylate

Inchi: InChI=1S/C6H7NO3/c1-2-9-6(8)5-3-4-7-10-5/h3-4H,2H2,1H3
InchiKey: JOWMDIFULFYASV-UHFFFAOYSA-N
Formula: C6H7NO3
SMILES: CCOC(=O)c1ccno1
Mol. weight [g/mol]: 141.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	0.851		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook

Sources

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=U375986&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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