

2-ethyl-3-formylthiophene

Other names: 2-Ethyl-3-carboxaldehyde-thiophene
Inchi: InChI=1S/C7H8OS/c1-2-7-6(5-8)3-4-9-7/h3-5H,2H2,1H3
InchiKey: BZJVXWRAUTYFQJ-UHFFFAOYSA-N
Formula: C7H8OS
SMILES: CCc1sccc1C=O
Mol. weight [g/mol]: 140.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	2.123		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1147.00		NIST Webbook
rinpol	1177.00		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=R282996&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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