2,3-Thiophenedicarboxylic acid

Inchi: InChI=1S/C6H4O4S/c7-5(8)3-1-2-11-4(3)6(9)10/h1-2H,(H,7,8)(H,9,10)
InchiKey: HIHKYDVSWLFRAY-UHFFFAOYSA-N
Formula: C6H4O4S
SMILES: O=C(O)c1ccsc1C(=O)O
Mol. weight [g/mol]: 172.16
CAS: 1451-95-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	1.145		Crippen Method
mcvol	107.170	ml/mol	McGowan Method
rinpol	1618.00		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=C1451952&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

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