

4-(2-Thienyl)butyric acid

Other names: 2-Thiophenebutanoic acid; 2-Thiophenebutyric acid; «gamma»-(«alpha»-Thienyl)butyric acid.

InChI: InChI=1S/C8H10O2S/c9-8(10)5-1-3-7-4-2-6-11-7/h2,4,6H,1,3,5H2,(H,9,10)

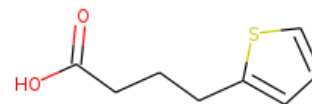
InChI Key: VYTXLSQVYGNWLV-UHFFFAOYSA-N

Formula: C8H10O2S

SMILES: O=C(O)CCCC1CCCS1

Molecular Weight: 170.23

CAS: 4653-11-6



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.16		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H10O2S/c9-8\(10\)5-1-3-7-4-2-6-11-7/h2,4,6H,1,3,5H2,\(H,9,10\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H10O2S/c9-8(10)5-1-3-7-4-2-6-11-7/h2,4,6H,1,3,5H2,(H,9,10))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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