2-Thiophenebutanoic acid, methyl ester

Other names:	Methyl 4-(2-thienyl)butanoate
	4-(2-Thienyl)butanoic acid methyl ester
Inchi:	InChI=1S/C9H12O2S/c1-11-9(10)6-2-4-8-5-3-7-12-8/h3,5,7H,2,4,6H2,1H3
InchiKey:	FUTXOYOSYBCRBT-UHFFFAOYSA-N
Formula:	C9H12O2S
SMILES:	COC(=O)CCCc1cccs1
Mol. weight [g/mol]:	184.25
CAS:	20828-66-4

Physical Properties

Property code	Value	Unit	Source
ie	8.40 ± 0.30	eV	NIST Webbook
log10ws	-2.15		Crippen Method
logp	2.244		Crippen Method
mcvol	142.000	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20828664&Units=SI
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

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from: