ethyl 2-thienylacetate

Other names:	Ethyl 2-thiopheneacetate
Inchi:	InChI=1S/C8H10O2S/c1-2-10-8(9)6-7-4-3-5-11-7/h3-5H,2,6H2,1H3
InchiKey:	QSUANHXENVRFDN-UHFFFAOYSA-N
Formula:	C8H10O2S
SMILES:	CCOC(=O)Cc1cccs1
Mol. weight [g/mol]:	170.23
CAS:	57382-97-5

Physical Properties

Property code	Value	Unit	Source
hvap	61.80 ± 1.30	kJ/mol	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.854		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
ripol	1998.00		NIST Webbook
ripol	1998.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Calorimetric study of methyl and ethyl 2-thiophenecarboxylates and ethyl 2- and 3-thiopheneacetates:	https://www.doi.org/10.1016/j.jct.2009.03.007
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57382975&Units=SI

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

ripol: Polar retention indices