

Methyl 2-thienylacetate

Other names:	2-Thiopheneacetic acid, methyl ester Methyl 2-thiopheneacetate Methyl thiophene-2-acetate methyl thiophen-2-acetate
Inchi:	InChI=1S/C7H8O2S/c1-9-7(8)5-6-3-2-4-10-6/h2-4H,5H2,1H3
InchiKey:	KNKIXYMOHMYZJR-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	COC(=O)Cc1cccs1
Mol. weight [g/mol]:	156.20
CAS:	19432-68-9

Physical Properties

Property code	Value	Unit	Source
cpl	249.80	J/molxK	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
hvap	61.90 ± 1.40	kJ/mol	NIST Webbook
log10ws	-1.31		Crippen Method
logp	1.464		Crippen Method
mcvol	113.820	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19432689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives:	https://www.doi.org/10.1016/j.tca.2005.11.024
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpl:	Liquid phase heat capacity
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

Latest version available from:

<https://www.cheméo.com/cid/96-960-0/Methyl-2-thienylacetate.pdf>

Generated by Cheméo on 2024-04-25 20:39:16.97851328 +0000 UTC m=+16366805.899090592.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.