

L-Alanine, N-(2-thienylcarbonyl)-, methyl ester

Inchi:	InChI=1S/C9H11NO3S/c1-6(9(12)13-2)10-8(11)7-4-3-5-14-7/h3-6H,1-2H3,(H,10,11)
InchiKey:	RGWBJRKEIGMOOW-UHFFFAOYSA-N
Formula:	C9H11NO3S
SMILES:	COC(=O)C(C)NC(=O)c1cccs1
Mol. weight [g/mol]:	213.26

Physical Properties

Property code	Value	Unit	Source
hvap	76.87	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
logp	1.039		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
rinpol	1649.00		NIST Webbook
tb	562.10	K	Cheméo Relay (1.0)
tf	374.85	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299594&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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