

L-Cysteine, N,S-bis(2-thienylcarbonyl)-, methyl ester

Inchi:	InChI=1S/C14H13NO4S3/c1-19-13(17)9(15-12(16)10-4-2-6-20-10)8-22-14(18)11-5-3-7-2
InchiKey:	ZATVPOXNRQMBGP-UHFFFAOYSA-N
Formula:	C14H13NO4S3
SMILES:	<chem>COC(=O)C(CSC(=O)c1cccs1)NC(=O)c1cccs1</chem>
Mol. weight [g/mol]:	355.46

Physical Properties

Property code	Value	Unit	Source
hvap	116.51	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
logp	2.655		Crippen Method
mcvol	238.810	ml/mol	McGowan Method
tb	670.81	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299600&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

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