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: COC(=O)C(CSC(=O)c1cccs1)NC(=O)c1cccs1

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.chemeo.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