l-Tyrosine, N,O-bis(2-thienylcarbonyl)-, methyl ester

Inchi: InChI=1S/C20H17NO5S2/c1-25-19(23)15(21-18(22)16-4-2-10-27-16)12-13-6-8-14(9-7-1
InchiKey: HWENSLXLUVVLFZ-UHFFFAOYSA-N
Formula: C20H17NO5S2
SMILES: COC(=O)C(Cc1ccc(OC(=O)c2cccs2)cc1)NC(=O)c1cccs1
Mol. weight [g/mol]: 415.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.26		Crippen Method
logp	3.543		Crippen Method
mcvol	289.110	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299601&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume