

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]: 415.49

Physical Properties

Property code	Value	Unit	Source
hvap	129.52	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	Cheméo Relay (1.0)
logp	3.543		Crippen Method
mcvol	289.110	ml/mol	McGowan Method
tb	716.86	K	Cheméo Relay (1.0)

Sources

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):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299601&Units=SI>

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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