l-Serine, N,O-bis(m-toluoyl)-, methyl ester

Inchi: InChI=1S/C20H21NO5/c1-13-6-4-8-15(10-13)18(22)21-17(20(24)25-3)12-26-19(23)16-9-
InchiKey: VXBKBULEELEDDO-UHFFFAOYSA-N
Formula: C20H21NO5
SMILES: COC(=O)C(COC(=O)c1cccc(C)c1)N=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 355.38

Physical Properties

Property code	Value	Unit	Source
hf	-580.69	kJ/mol	Joback Method
hvap	103.99	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.007		Crippen Method
mcvol	271.570	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
tb	1041.20	K	Joback Method
tc	1280.59	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299644&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature