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)NC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 355.39

Physical Properties

Property code	Value	Unit	Source
hf	-726.45	kJ/mol	Cheméo Relay (1.0)
hfus	43.61	kJ/mol	Joback Method
hvap	124.79	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-4.40		Cheméo Relay (1.0)
logp	2.432		Crippen Method
mcvol	271.570	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	676.35	K	Cheméo Relay (1.0)
tc	962.34	K	Cheméo Relay (1.0)
tf	340.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.90	J/mol×K	976.50	Joback Method
cpg	853.64	J/mol×K	1015.73	Joback Method
cpg	862.97	J/mol×K	1054.96	Joback Method
cpg	870.93	J/mol×K	1094.18	Joback Method
cpg	877.55	J/mol×K	1133.41	Joback Method
cpg	882.88	J/mol×K	1172.64	Joback Method
cpg	886.95	J/mol×K	1211.87	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299644&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point