L-Serine, N,O-bis(4-fluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C18H15F2NO5/c1-25-18(24)15(21-16(22)11-2-6-13(19)7-3-11)10-26-17(23)12
InchiKey: GOKLUIQFDJMZMZ-UHFFFAOYSA-N
Formula: C18H15F2NO5
SMILES: COC(=O)C(COC(=O)c1ccc(F)cc1)NC(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 363.32

Physical Properties

Property code	Value	Unit	Source
hfus	44.59	kJ/mol	Joback Method
logp	2.093		Crippen Method
mcvol	246.930	ml/mol	McGowan Method
rinpol	2466.00		NIST Webbook
tb	663.60	K	Cheméo Relay (1.0)
tf	352.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.90	J/mol×K	929.28	Joback Method
cpg	752.78	J/mol×K	966.92	Joback Method
cpg	761.45	J/mol×K	1004.56	Joback Method
cpg	768.91	J/mol×K	1042.20	Joback Method
cpg	775.20	J/mol×K	1079.84	Joback Method
cpg	780.35	J/mol×K	1117.48	Joback Method
cpg	784.39	J/mol×K	1155.12	Joback Method

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=U299609&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point