l-Serine, N,O-bis(3-fluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C18H15F2NO5/c1-25-18(24)15(21-16(22)11-4-2-6-13(19)8-11)10-26-17(23)12
InchiKey: PTXSJEPNTGOUHE-UHFFFAOYSA-N
Formula: C18H15F2NO5
SMILES: COC(=O)C(COC(=O)c1cccc(F)c1)NC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 363.31

Physical Properties

Property code	Value	Unit	Source
gf	-593.19	kJ/mol	Joback Method
hf	-910.94	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	2.093		Crippen Method
mcvol	246.930	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	929.28	K	Joback Method
tc	1155.12	K	Joback Method
tf	603.59	K	Joback Method
vc	0.947	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U299680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume