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

Inchi: InChI=1S/C20H15F6NO5/c1-31-18(30)15(27-16(28)11-4-2-6-13(8-11)19(21,22)23)10-32
InchiKey: VSVQKHPVTGRBJT-UHFFFAOYSA-N
Formula: C20H15F6NO5
SMILES: COC(=O)C(COC(=O)c1cccc(C(F)(F)F)c1)NC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 463.33

Physical Properties

Property code	Value	Unit	Source
gf	-1349.91	kJ/mol	Joback Method
hf	-1754.16	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	3.853		Crippen Method
mcvol	282.190	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2322.00		NIST Webbook
tb	965.66	K	Joback Method
tc	1186.35	K	Joback Method
tf	633.33	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.14	J/mol×K	965.66	Joback Method
cpg	895.45	J/mol×K	1002.44	Joback Method
cpg	903.75	J/mol×K	1039.22	Joback Method
cpg	911.13	J/mol×K	1076.00	Joback Method
cpg	917.68	J/mol×K	1112.79	Joback Method
cpg	923.47	J/mol×K	1149.57	Joback Method
cpg	928.60	J/mol×K	1186.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299703&Units=SI

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