l-Serine, N,O-bis(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C18H11F6NO5/c1-29-18(28)11(25-16(26)7-2-4-9(19)14(23)12(7)21)6-30-17(2

InchiKey: PBVWNLNSUIDONC-UHFFFAOYSA-N

Formula: C18H11F6NO5

SMILES: COC(=O)C(COC(=O)c1ccc(F)c(F)c1F)NC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 435.27

Physical Properties

Property code	Value	Unit	Source
gf	-1410.95	kJ/mol	Joback Method
hf	-1741.26	kJ/mol	Joback Method
hfus	55.35	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	2.650		Crippen Method
mcvol	254.010	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2333.00		NIST Webbook
tb	946.28	K	Joback Method
tc	1161.04	K	Joback Method
tf	656.03	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.49	J/mol×K	946.28	Joback Method
cpg	772.84	J/mol×K	982.07	Joback Method
cpg	780.02	J/mol×K	1017.87	Joback Method
cpg	786.04	J/mol×K	1053.66	Joback Method
cpg	790.91	J/mol×K	1089.46	Joback Method
cpg	794.62	J/mol×K	1125.25	Joback Method
cpg	797.19	J/mol×K	1161.04	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=U299634&Units=SI
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
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