l-Serine, N,O-bis-(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C18H13F4NO5/c1-27-17(25)13(23-16(24)14-9(19)4-2-5-10(14)20)8-28-18(26)1
InchiKey: FKFQYFNFXJNQEB-UHFFFAOYSA-N
Formula: C18H13F4NO5
SMILES: COC(=O)C(COC(=O)c1c(F)cccc1F)NC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 399.29

Physical Properties

Property code	Value	Unit	Source
gf	-1002.07	kJ/mol	Joback Method
hf	-1326.10	kJ/mol	Joback Method
hfus	49.97	kJ/mol	Joback Method
hvap	90.70	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	2.371		Crippen Method
mcvol	250.470	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	937.78	K	Joback Method
tc	1156.41	K	Joback Method
tf	629.81	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.79	J/mol×K	937.78	Joback Method
cpg	762.83	J/mol×K	974.22	Joback Method
cpg	770.70	J/mol×K	1010.66	Joback Method
cpg	777.41	J/mol×K	1047.10	Joback Method
cpg	782.97	J/mol×K	1083.54	Joback Method
cpg	787.40	J/mol×K	1119.97	Joback Method
cpg	790.71	J/mol×K	1156.41	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=U299665&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