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

Inchi: InChI=1S/C26H19F6NO5/c1-37-24(36)21(33-22(34)16-4-2-6-18(13-16)25(27,28)29)12-1

InchiKey: ZYUOSULCYXWEKZ-UHFFFAOYSA-N

Formula: C26H19F6NO5

SMILES: COC(=O)C(Cc1ccc(OC(=O)c2cccc(C(F)(F)F)c2)cc1)NC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 539.42

Physical Properties

Property code	Value	Unit	Source
gf	-1196.61	kJ/mol	Joback Method
hf	-1652.94	kJ/mol	Joback Method
hfus	56.45	kJ/mol	Joback Method
hvap	105.90	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	5.458		Crippen Method
mcvol	342.970	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
tb	1134.60	K	Joback Method
tc	1389.18	K	Joback Method
tf	739.89	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.95	J/mol×K	1134.60	Joback Method
cpg	1125.17	J/mol×K	1177.03	Joback Method
cpg	1132.45	J/mol×K	1219.46	Joback Method
cpg	1138.95	J/mol×K	1261.89	Joback Method
cpg	1144.84	J/mol×K	1304.32	Joback Method
cpg	1150.27	J/mol×K	1346.75	Joback Method
cpg	1155.40	J/mol×K	1389.18	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=U299705&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume