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

Inchi: InChI=1S/C24H17F4NO5/c1-33-23(31)19(29-22(30)20-15(25)4-2-5-16(20)26)12-13-8-10

InchiKey: OEONJOSRYODGNS-UHFFFAOYSA-N

Formula: C24H17F4NO5

SMILES: COC(=O)C(Cc1ccc(OC(=O)c2c(F)cccc2F)cc1)NC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 475.39

Physical Properties

Property code	Value	Unit	Source
gf	-848.77	kJ/mol	Joback Method
hf	-1224.88	kJ/mol	Joback Method
hfus	59.16	kJ/mol	Joback Method
hvap	106.99	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	3.976		Crippen Method
mcvol	311.250	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
tb	1106.72	K	Joback Method
tc	1355.32	K	Joback Method
tf	736.37	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.23	J/mol×K	1106.72	Joback Method
cpg	986.49	J/mol×K	1148.15	Joback Method
cpg	991.17	J/mol×K	1189.59	Joback Method
cpg	994.32	J/mol×K	1231.02	Joback Method
cpg	996.00	J/mol×K	1272.45	Joback Method
cpg	996.26	J/mol×K	1313.89	Joback Method
cpg	995.16	J/mol×K	1355.32	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=U299667&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume