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
hfus	59.16	kJ/mol	Joback Method
logp	3.976		Crippen Method
mcvol	311.250	ml/mol	McGowan 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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299667&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume