

L-Tyrosine, N,O-bis(2-trifluoromethylbenzoyl)-, methyl ester

InChI: InChI=1S/C26H19F6NO5/c1-37-24(36)21(33-22(34)17-6-2-4-8-19(17)25(27,28)29)14-15

InChIKey: MTXLVTBNDCCFFIM-UHFFFAOYSA-N

Formula: C26H19F6NO5

SMILES: COC(=O)C(Cc1ccc(OC(=O)c2ccccc2C(F)(F)F)cc1)NC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 539.43

Physical Properties

Property code	Value	Unit	Source
hfus	56.45	kJ/mol	Joback Method
logp	5.458		Crippen Method
mcvol	342.970	ml/mol	McGowan 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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299691&Units=SI>

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

Legend

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

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