

L-Tyrosine, N,O-bis(3-fluorobenzoyl)-, methyl ester

Inchi:	InChI=1S/C24H19F2NO5/c1-31-24(30)21(27-22(28)16-4-2-6-18(25)13-16)12-15-8-10-20
InchiKey:	BDTBDTZRJXWVLY-UHFFFAOYSA-N
Formula:	C24H19F2NO5
SMILES:	COC(=O)C(Cc1ccc(OC(=O)c2cccc(F)c2)cc1)NC(=O)c1cccc(F)c1
Mol. weight [g/mol]:	439.41

Physical Properties

Property code	Value	Unit	Source
hfus	53.78	kJ/mol	Joback Method
logp	3.698		Crippen Method
mcvol	307.710	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.72	J/mol×K	1098.22	Joback Method
cpg	978.91	J/mol×K	1139.95	Joback Method
cpg	984.61	J/mol×K	1181.68	Joback Method
cpg	988.88	J/mol×K	1223.41	Joback Method
cpg	991.78	J/mol×K	1265.13	Joback Method
cpg	993.39	J/mol×K	1306.86	Joback Method
cpg	993.78	J/mol×K	1348.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299682&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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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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