

L-Tyrosine, N,O-bis(pivaloyl)-, methyl ester

Inchi: InChI=1S/C20H29NO5/c1-19(2,3)17(23)21-15(16(22)25-7)12-13-8-10-14(11-9-13)26-18
InchiKey: BLWCXJZLBUEQQH-UHFFFAOYSA-N
Formula: C20H29NO5
SMILES: COC(=O)C(Cc1ccc(OC(=O)C(C)(C)C)cc1)N=C(O)C(C)(C)C
Mol. weight [g/mol]: 363.45

Physical Properties

Property code	Value	Unit	Source
hf	-823.25	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.725		Crippen Method
mcvol	295.330	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	1003.08	K	Joback Method
tc	1232.26	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299750&Units=SI>
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>

Legend

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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