l-Tyrosine, N,O-bis(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C26H37NO5/c1-31-26(30)23(27-24(28)16-12-19-6-2-3-7-19)18-21-10-14-22(15

InchiKey: JXGANONFBSEACI-UHFFFAOYSA-N

Formula: C26H37NO5

SMILES: COC(=O)C(Cc1ccc(OC(=O)CCC2CCCC2)cc1)NC(=O)CCC1CCCC1

Mol. weight [g/mol]: 443.58

Physical Properties

Property code	Value	Unit	Source
gf	-165.89	kJ/mol	Joback Method
hf	-787.94	kJ/mol	Joback Method
hfus	53.37	kJ/mol	Joback Method
hvap	108.03	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	4.733		Crippen Method
mcvol	358.150	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
tb	1112.68	K	Joback Method
tc	1362.59	K	Joback Method
tf	675.43	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.09	J/mol×K	1112.68	Joback Method
cpg	1303.69	J/mol×K	1154.33	Joback Method
cpg	1314.51	J/mol×K	1195.98	Joback Method
cpg	1323.65	J/mol×K	1237.63	Joback Method
cpg	1331.23	J/mol×K	1279.29	Joback Method
cpg	1337.36	J/mol×K	1320.94	Joback Method
cpg	1342.13	J/mol×K	1362.59	Joback Method

Sources

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=U299659&Units=SI
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
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

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