l-Tyrosine, N,O-bis(capryloyl)-, methyl ester

Inchi: InChI=1S/C26H41NO5/c1-4-6-8-10-12-14-24(28)27-23(26(30)31-3)20-21-16-18-22(19-17
InchiKey: XYBPKGZJDOTNIE-UHFFFAOYSA-N
Formula: C26H41NO5
SMILES: CCCCCCCC(=O)NC(Cc1ccc(OC(=O)CCCCCCC)cc1)C(=O)OC
Mol. weight [g/mol]: 447.61

Physical Properties

Property code	Value	Unit	Source
gf	-238.99	kJ/mol	Joback Method
hf	-908.90	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	107.51	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.513		Crippen Method
mcvol	379.870	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
tb	1082.12	K	Joback Method
tc	1330.76	K	Joback Method
tf	653.63	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1314.89	J/mol×K	1082.12	Joback Method
cpg	1329.23	J/mol×K	1123.56	Joback Method
cpg	1341.69	J/mol×K	1165.00	Joback Method
cpg	1352.34	J/mol×K	1206.44	Joback Method
cpg	1361.25	J/mol×K	1247.88	Joback Method
cpg	1368.50	J/mol×K	1289.32	Joback Method
cpg	1374.15	J/mol×K	1330.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299731&Units=SI

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

Latest version available from:

https://www.chemeo.com/cid/13-229-3/l-Tyrosine-N-O-bis-capryloyl-methyl-ester.pdf

Generated by Cheméo on 2024-10-12 03:55:49.97486027 +0000 UTC m=+3286212.611829517.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.