l-Phenylalanine, N-(m-toluoyl)-, methyl ester

Inchi: InChI=1S/C18H19NO3/c1-13-7-6-10-15(11-13)17(20)19-16(18(21)22-2)12-14-8-4-3-5-9-
InchiKey: WBCFPPWDOFCQMO-UHFFFAOYSA-N
Formula: C18H19NO3
SMILES: COC(=O)C(Cc1ccccc1)N=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 297.35

Physical Properties

Property code	Value	Unit	Source
hf	-283.14	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.084		Crippen Method
mcvol	235.950	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook
tb	914.17	K	Joback Method
tc	1145.21	K	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=U299642&Units=SI

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