

L-Phenylalanine, N-(m-anisoyl)-, methyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H19NO4/c1-22-15-10-6-9-14(12-15)17(20)19-16(18(21)23-2)11-13-7-4-3-5

KKEYBYFADKWFPE-UHFFFAOYSA-N

C18H19NO4

COC(=O)C(Cc1ccccc1)NC(=O)c1cccc(OC)c1

313.35

Physical Properties

Property code	Value	Unit	Source
hf	-474.15	kJ/mol	Cheméo Relay (1.0)
hfus	37.22	kJ/mol	Joback Method
hvap	115.16	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-3.73		Cheméo Relay (1.0)
logp	2.209		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
rinpol	2544.00		NIST Webbook
tb	657.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.11	J/mol×K	871.89	Joback Method
cpg	735.12	J/mol×K	910.48	Joback Method
cpg	746.83	J/mol×K	949.07	Joback Method
cpg	757.26	J/mol×K	987.65	Joback Method
cpg	766.47	J/mol×K	1026.24	Joback Method
cpg	774.48	J/mol×K	1064.83	Joback Method
cpg	781.34	J/mol×K	1103.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299712&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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