Phenylalanine-N-carboxylic acid dimethyl ester

Inchi: InChI=1S/C12H15NO4/c1-16-11(14)10(13-12(15)17-2)8-9-6-4-3-5-7-9/h3-7,10H,8H2,1-2

InchiKey: JIHFRPSFLTXYEP-UHFFFAOYSA-N

Formula: C12H15NO4

SMILES: COC(=O)C(Cc1ccccc1)N=C(O)OC

Mol. weight [g/mol]: 237.25

CAS: 70288-75-4

Physical Properties

Property code	Value	Unit	Source
chs	-6099.40 ± 5.90	kJ/mol	NIST Webbook
hf	-516.58	kJ/mol	Joback Method
hfs	-766.40 ± 5.90	kJ/mol	NIST Webbook
hvap	75.83	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.331		Crippen Method
mcvol	181.040	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	767.65	K	Joback Method
tc	979.00	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=C70288754&Units=SI

Legend

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature