2-Phenylacetylamino-pentanedioic acid dimethyl ester

Inchi: InChI=1S/C15H17NO5/c1-20-14(18)9-8-12(15(19)21-2)16-13(17)10-11-6-4-3-5-7-11/h3-8

InchiKey: QUAHCOYCPGQAMQ-WQLSENKSSA-N

Formula: C15H17NO5

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

Mol. weight [g/mol]: 291.30

Physical Properties

Property code	Value	Unit	Source
hf	-578.37	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.806		Crippen Method
mcvol	220.580	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	894.64	K	Joback Method
tc	1113.54	K	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=R247819&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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