Pentanedioic acid, 2-(phenylacetylamino(, dimethyl ester

Inchi: InChI=1S/C15H19NO5/c1-20-14(18)9-8-12(15(19)21-2)16-13(17)10-11-6-4-3-5-7-11/h3-7

InchiKey: FXBCZQJEDNRALO-UHFFFAOYSA-N

Formula: C15H19NO5

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

Mol. weight [g/mol]: 293.32

Physical Properties

Property code	Value	Unit	Source
hf	-691.08	kJ/mol	Joback Method
hvap	89.26	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	1.680		Crippen Method
mcvol	224.880	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2173.00		NIST Webbook
rinpol	2173.00		NIST Webbook
tb	890.16	K	Joback Method
tc	1104.72	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R106679&Units=SI

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

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