

Phenyl 1,2-dicarbethoxyethylcarbamate

Inchi: InChI=1S/C15H19NO6/c1-3-20-13(17)10-12(14(18)21-4-2)16-15(19)22-11-8-6-5-7-9-11/
InchiKey: JIDYZYNLVLTRR-UHFFFAOYSA-N
Formula: C15H19NO6
SMILES: CCOC(=O)CC(N=C(O)Oc1ccccc1)C(=O)OCC
Mol. weight [g/mol]: 309.31

Physical Properties

Property code	Value	Unit	Source
hf	-823.30	kJ/mol	Joback Method
hvap	91.67	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.864		Crippen Method
mcvol	230.750	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
tb	912.58	K	Joback Method
tc	1128.00	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=B6002175&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

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