Methyl phenethylcarbamate

Inchi: InChI=1S/C10H13NO2/c1-13-10(12)11-8-7-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H,11,12)
InchiKey: QIWRMPPFDARXPF-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: COC(O)=NCCc1ccccc1
Mol. weight [g/mol]: 179.22
CAS: 26011-68-7

Physical Properties

Property code	Value	Unit	Source
hf	-225.22	kJ/mol	Joback Method
hvap	62.61	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.790		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1496.30		NIST Webbook
rinpol	1496.30		NIST Webbook
tb	646.04	K	Joback Method
tc	854.89	K	Joback Method

Sources

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=C26011687&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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