

Phenethyl carbamic acid, ethyl ester

Inchi:	InChI=1S/C11H15NO2/c1-2-14-11(13)12-9-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,
InchiKey:	WXDDBYFBIAYSM-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CCOC(O)=NCCc1ccccc1
Mol. weight [g/mol]:	193.24
CAS:	6970-83-8

Physical Properties

Property code	Value	Unit	Source
hf	-245.86	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.180		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	668.92	K	Joback Method
tc	874.77	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6970838&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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