

Carbamic acid, phenyl-, propyl ester

Other names:	Carbanilic acid, propyl ester Propyl carbanilate Propyl phenylcarbamate Propyl phenylurethane Propyl N-phenylcarbamate Carbanilic acid, n-propyl ester
Inchi:	InChI=1S/C10H13NO2/c1-2-8-13-10(12)11-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,11,12)
InchiKey:	QDZXCXBFZLLQFT-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCCOC(O)=Nc1ccccc1
Mol. weight [g/mol]:	179.22
CAS:	5532-90-1

Physical Properties

Property code	Value	Unit	Source
hf	-225.22	kJ/mol	Joback Method
hvap	62.61	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.659		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1483.00		NIST Webbook
ripol	2113.00		NIST Webbook
tb	646.04	K	Joback Method
tc	854.89	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5532901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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