

Phenylacetamide, N-propyl-

Inchi:	InChI=1S/C11H15NO/c1-2-8-12-11(13)9-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,13)
InchiKey:	HTSYYPRWWXXRSC-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CCCN=C(O)Cc1ccccc1
Mol. weight [g/mol]:	177.24

Physical Properties

Property code	Value	Unit	Source
hf	-113.64	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.596		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1596.00		NIST Webbook
rinpol	1596.00		NIST Webbook
tb	646.50	K	Joback Method
tc	854.33	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407221&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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