

Phenylacetamide, N-ethyl-

Inchi:	InChI=1S/C10H13NO/c1-2-11-10(12)8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,11,12)
InchiKey:	QDHFDXDMKYJPSC-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CCN=C(O)Cc1ccccc1
Mol. weight [g/mol]:	163.22

Physical Properties

Property code	Value	Unit	Source
hf	-93.00	kJ/mol	Joback Method
hvap	60.20	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.206		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	623.62	K	Joback Method
tc	834.71	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407220&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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