

1-Propanamine, N-(phenylmethylene)-

Other names:	Propylamine, N-benzylidene- N-Benzylidenepropylamine N-(Phenylmethyldene)-1-propanamine Benzylidene-propyl-amine N-Propylbenzylideneimine
Inchi:	InChI=1S/C10H13N/c1-2-8-11-9-10-6-4-3-5-7-10/h3-7,9H,2,8H2,1H3
InchiKey:	DFROALYLRQTARX-UHFFFAOYSA-N
Formula:	C10H13N
SMILES:	CCCN=Cc1ccccc1
Mol. weight [g/mol]:	147.22
CAS:	6852-55-7

Physical Properties

Property code	Value	Unit	Source
hf	69.02	kJ/mol	Joback Method
hvap	43.44	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.516		Crippen Method
mcvol	133.680	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1777.00		NIST Webbook
tb	531.56	K	Joback Method
tc	755.80	K	Joback Method

Sources

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=C6852557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	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
r_{in}pol:	Non-polar retention indices
r_pol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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