

Phenylacetamide, N-nonyl-

Inchi:	InChI=1S/C17H27NO/c1-2-3-4-5-6-7-11-14-18-17(19)15-16-12-9-8-10-13-16/h8-10,12-13
InchiKey:	TYBVVSYINSQHHY-UHFFFAOYSA-N
Formula:	C17H27NO
SMILES:	CCCCCCCCCN=C(O)Cc1ccccc1
Mol. weight [g/mol]:	261.40

Physical Properties

Property code	Value	Unit	Source
hf	-237.48	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.936		Crippen Method
mcpvol	238.180	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	783.78	K	Joback Method
tc	980.39	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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