

N-phenethylnonanamide

Inchi:	InChI=1S/C17H27NO/c1-2-3-4-5-6-10-13-17(19)18-15-14-16-11-8-7-9-12-16/h7-9,11-12
InchiKey:	DEBIRUJQYICIMKU-UHFFFAOYSA-N
Formula:	C17H27NO
SMILES:	CCCCCCCCC(O)=NCCc1ccccc1
Mol. weight [g/mol]:	261.40
CAS:	560089-64-7

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
mcvol	238.180	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2203.90		NIST Webbook
rinpol	2203.90		NIST Webbook
tb	783.78	K	Joback Method
tc	980.39	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=C560089647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
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h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{npol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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