

Benzamide, 3-methyl-N-nonyl-

Inchi:	InChI=1S/C17H27NO/c1-3-4-5-6-7-8-9-13-18-17(19)16-12-10-11-15(2)14-16/h10-12,14H
InchiKey:	FKTLHVWWECIUBI-UHFFFAOYSA-N
Formula:	C17H27NO
SMILES:	CCCCCCCCCN=C(O)c1cccc(C)c1
Mol. weight [g/mol]:	261.40

Physical Properties

Property code	Value	Unit	Source
hf	-248.95	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.050		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	788.76	K	Joback Method
tc	986.19	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=U407419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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