

N,N-Dimethyl-N'-nonyl-benzamide

Inchi:	InChI=1S/C18H30N2/c1-4-5-6-7-8-9-13-16-19-18(20(2)3)17-14-11-10-12-15-17/h10-12,1
InchiKey:	LKCIHOGRQQYWSC-VHEBQXMUSA-N
Formula:	C18H30N2
SMILES:	CCCCCCCCCN=C(c1ccccc1)N(C)C
Mol. weight [g/mol]:	274.44

Physical Properties

Property code	Value	Unit	Source
hf	-38.36	kJ/mol	Joback Method
hvap	63.38	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.745		Crippen Method
mcpvol	256.380	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	726.92	K	Joback Method
tc	926.54	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R159292&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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