

N,N-Dimethyl-2-phenyl-N'-octyl-acetamide

Inchi: InChI=1S/C18H30N2/c1-4-5-6-7-8-12-15-19-18(20(2)3)16-17-13-10-9-11-14-17/h9-11,13
InchiKey: WQICHHSOPJGGKR-VHEBQXMUSA-N
Formula: C18H30N2
SMILES: CCCCCCN=C(Cc1ccccc1)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	-4.69		Crippen Method
logp	4.550		Crippen Method
mcvol	256.380	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinsol	2072.00		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=R162317&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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