

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

Inchi: InChI=1S/C13H20N2/c1-4-10-14-13(15(2)3)11-12-8-6-5-7-9-12/h5-9H,4,10-11H2,1-3H3/
InchiKey: RTOIWWYNCPAZHX-BUHFOSPRSA-N
Formula: C13H20N2
SMILES: CCCN=C(Cc1ccccc1)N(C)C
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
hf	64.84	kJ/mol	Joback Method
hvap	52.25	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.599		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1605.00		NIST Webbook
tb	612.52	K	Joback Method
tc	825.86	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=R162342&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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