

N,N-Dimethyl-2-phenyl-N'-(3-methoxyphenyl)-acet

Inchi: InChI=1S/C17H20N2O/c1-19(2)17(12-14-8-5-4-6-9-14)18-15-10-7-11-16(13-15)20-3/h4-
InchiKey: MMBKEBZBGRKISP-ISLYRVAYSA-N
Formula: C17H20N2O
SMILES: COc1cccc(N=C(Cc2ccccc2)N(C)C)c1
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
hf	75.12	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.529		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	1854.71	kPa	Joback Method
rinpol	2272.00		NIST Webbook
tb	758.12	K	Joback Method
tc	994.66	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=R162159&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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