

N'-(3-methoxy-phenyl)-N,N-dimethyl-acetamide

Inchi: InChI=1S/C11H16N2O/c1-9(13(2)3)12-10-6-5-7-11(8-10)14-4/h5-8H,1-4H3
InchiKey: UMCNCQPROLZHTL-UHFFFAOYSA-N
Formula: C11H16N2O
SMILES: COc1cccc(N=C(C)N(C)C)c1
Mol. weight [g/mol]: 192.26

Physical Properties

Property code	Value	Unit	Source
hf	-37.57	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.307		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinsol	1687.00		NIST Webbook
rinsol	1687.00		NIST Webbook
tb	594.16	K	Joback Method
tc	813.37	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R153294&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

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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