N,N-Dimethyl-N'-(3-methoxyphenyl)-isobutyramid

Inchi: InChI=1S/C13H20N2O/c1-10(2)13(15(3)4)14-11-7-6-8-12(9-11)16-5/h6-10H,1-5H3
InchiKey: PBUBOAHQRYABAY-UHFFFAOYSA-N
Formula: C13H20N2O
SMILES: COc1cccc(N=C(C(C)C)N(C)C)c1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
hf	-84.13	kJ/mol	Joback Method
hvap	54.93	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.943		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook
tb	639.48	K	Joback Method
tc	855.52	K	Joback Method

Sources

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=R162411&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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