

N,N-Dimethyl-N'-(3-ethoxyphenyl)-isobutyramidin

Inchi: InChI=1S/C14H22N2O/c1-6-17-13-9-7-8-12(10-13)15-14(11(2)3)16(4)5/h7-11H,6H2,1-5H
InchiKey: JRKWZKADAFDTQM-UHFFFAOYSA-N
Formula: C14H22N2O
SMILES: CCOc1cccc(N=C(C(C)C)N(C)C)c1
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
hf	-104.77	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.333		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	662.36	K	Joback Method
tc	874.89	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162397&Units=SI>

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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