

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

Inchi:	InChI=1S/C13H20N2/c1-10(2)13(15(4)5)14-12-8-6-7-11(3)9-12/h6-10H,1-5H3/b14-13+
InchiKey:	MHJHLKPQFACWMK-BUHFOSPRSA-N
Formula:	C13H20N2
SMILES:	<chem>Cc1cccc(N=C(C(C)C)N(C)C)c1</chem>
Mol. weight [g/mol]:	204.31

Physical Properties

Property code	Value	Unit	Source
hf	48.09	kJ/mol	Joback Method
hvap	52.52	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.243		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1615.00		NIST Webbook
rinpol	1615.00		NIST Webbook
tb	617.06	K	Joback Method
tc	835.73	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R162431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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