

N,N-Dimethyl-N'-heptyl-isobutyramidine

Inchi: InChI=1S/C13H28N2/c1-6-7-8-9-10-11-14-13(12(2)3)15(4)5/h12H,6-11H2,1-5H3/b14-13
InchiKey: CWPCNOFREFHUHV-BUHFOSPRSA-N
Formula: C13H28N2
SMILES: CCCCCCN=C(C(C)C)N(C)C
Mol. weight [g/mol]: 212.37

Physical Properties

Property code	Value	Unit	Source
hf	-176.97	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.573		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinsol	1485.00		NIST Webbook
tb	585.40	K	Joback Method
tc	765.45	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R162679&Units=SI>
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>

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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