

N,N-Dimethyl-N'-hexyl-propionamide

Inchi: InChI=1S/C11H24N2/c1-5-7-8-9-10-12-11(6-2)13(3)4/h5-10H2,1-4H3/b12-11+
InchiKey: CEEDNSXFGDTPON-VAWYXSNFSA-N
Formula: C11H24N2
SMILES: CCCCCCN=C(CC)N(C)C
Mol. weight [g/mol]: 184.32

Physical Properties

Property code	Value	Unit	Source
hf	-130.41	kJ/mol	Joback Method
hvap	45.52	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.937		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1366.00		NIST Webbook
tb	540.08	K	Joback Method
tc	720.17	K	Joback Method

Sources

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=R162055&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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