

N,N-Dimethyl-N'-octyl-propionamide

Inchi:	InChI=1S/C13H28N2/c1-5-7-8-9-10-11-12-14-13(6-2)15(3)4/h5-12H2,1-4H3
InchiKey:	UKISWUKKGLMKJY-UHFFFAOYSA-N
Formula:	C13H28N2
SMILES:	CCCCCCCCN=C(CC)N(C)C
Mol. weight [g/mol]:	212.37

Physical Properties

Property code	Value	Unit	Source
hf	-171.69	kJ/mol	Joback Method
hvap	49.97	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.717		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1550.00		NIST Webbook
tb	585.84	K	Joback Method
tc	762.76	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R162075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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