

Acetamide, N-octyl-

Inchi:	InChI=1S/C10H21NO/c1-3-4-5-6-7-8-9-11-10(2)12/h3-9H2,1-2H3,(H,11,12)
InchiKey:	GLJKLMQZANYKBO-UHFFFAOYSA-N
Formula:	C10H21NO
SMILES:	CCCCCCCCN=C(C)O
Mol. weight [g/mol]:	171.28

Physical Properties

Property code	Value	Unit	Source
hf	-329.53	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.323		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1508.00		NIST Webbook
tb	596.94	K	Joback Method
tc	772.83	K	Joback Method

Sources

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=U406527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/78-774-7/Acetamide-N-octyl.pdf>

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