

# Acetoacetamide, n-(1,1,3,3-tetramethylbutyl)-

<b>Inchi:</b>	InChI=1S/C12H23NO2/c1-9(14)7-10(15)13-12(5,6)8-11(2,3)4/h7-8H2,1-6H3,(H,13,15)
<b>InchiKey:</b>	ROXIBSLHIBBFKK-UHFFFAOYSA-N
<b>Formula:</b>	C12H23NO2
<b>SMILES:</b>	CC(=O)CC(=O)NC(C)(C)CC(C)(C)C
<b>Mol. weight [g/mol]:</b>	213.32
<b>CAS:</b>	116346-20-4

## Physical Properties

Property code	Value	Unit	Source
gf	-112.61	kJ/mol	Joback Method
hf	-480.20	kJ/mol	Joback Method
hfus	20.31	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.296		Crippen Method
mcvol	193.060	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	625.41	K	Joback Method
tc	824.40	K	Joback Method
tf	382.36	K	Joback Method
vc	0.733	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.66	J/molxK	625.41	Joback Method
cpg	538.70	J/molxK	658.57	Joback Method
cpg	553.75	J/molxK	691.74	Joback Method
cpg	567.85	J/molxK	724.90	Joback Method
cpg	581.07	J/molxK	758.07	Joback Method
cpg	593.46	J/molxK	791.23	Joback Method
cpg	605.09	J/molxK	824.40	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346204&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346204&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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