

# Acetoxyacetamide, N-ethyl-N-(3-methylphenyl)-

Inchi:	InChI=1S/C13H17NO3/c1-4-14(13(16)9-17-11(3)15)12-7-5-6-10(2)8-12/h5-8H,4,9H2,1-3
InchiKey:	DUCYWABKWIKBRX-UHFFFAOYSA-N
Formula:	C13H17NO3
SMILES:	CCN(C(=O)COC(C)=O)c1cccc(C)c1
Mol. weight [g/mol]:	235.28

## Physical Properties

Property code	Value	Unit	Source
gf	-90.70	kJ/mol	Joback Method
hf	-376.44	kJ/mol	Joback Method
hfus	30.48	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.911		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	671.10	K	Joback Method
tc	879.20	K	Joback Method
tf	429.77	K	Joback Method
vc	0.704	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.97	J/mol×K	671.10	Joback Method
cpg	514.45	J/mol×K	705.78	Joback Method
cpg	528.00	J/mol×K	740.47	Joback Method
cpg	540.67	J/mol×K	775.15	Joback Method
cpg	552.47	J/mol×K	809.83	Joback Method
cpg	563.43	J/mol×K	844.52	Joback Method
cpg	573.58	J/mol×K	879.20	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=U308292&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308292&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpola:</b>	Non-polar retention indices
<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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