

# 3',4'-Methylenedioxyacetanilide

<b>Inchi:</b>	InChI=1S/C9H9NO3/c1-6(11)10-7-2-3-8-9(4-7)13-5-12-8/h2-4H,5H2,1H3,(H,10,11)
<b>InchiKey:</b>	CGLCDOZYDURWIG-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO3
<b>SMILES:</b>	CC(=O)Nc1ccc2c(c1)OCO2
<b>Mol. weight [g/mol]:</b>	179.17
<b>CAS:</b>	13067-19-1

## Physical Properties

Property code	Value	Unit	Source
gf	-25.26	kJ/mol	Joback Method
hf	-245.47	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	61.65	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.374		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	611.31	K	Joback Method
tc	843.75	K	Joback Method
tf	420.56	K	Joback Method
vc	0.472	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.72	J/molxK	611.31	Joback Method
cpg	326.00	J/molxK	650.05	Joback Method
cpg	336.43	J/molxK	688.79	Joback Method
cpg	346.07	J/molxK	727.53	Joback Method
cpg	354.98	J/molxK	766.27	Joback Method
cpg	363.24	J/molxK	805.01	Joback Method
cpg	370.90	J/molxK	843.75	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=C13067191&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13067191&amp;Units=SI</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>mccvol:</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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