

# 3-(CH3)2NC6H4COOCH3

**Inchi:** InChI=1S/C10H13NO2/c1-11(2)9-6-4-5-8(7-9)10(12)13-3/h4-7H,1-3H3  
**InchiKey:** CABFTHPIDKWPNQ-UHFFFAOYSA-N  
**Formula:** C10H13NO2  
**SMILES:** COC(=O)c1cccc(N(C)C)c1  
**Mol. weight [g/mol]:** 179.22  
**CAS:** 16518-64-2

## Physical Properties

Property code	Value	Unit	Source
affp	930.20	kJ/mol	NIST Webbook
basg	903.80	kJ/mol	NIST Webbook
gf	12.96	kJ/mol	Joback Method
hf	-201.94	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	51.99	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.539		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	548.59	K	Joback Method
tc	759.30	K	Joback Method
tf	346.03	K	Joback Method
vc	0.529	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.56	J/molxK	548.59	Joback Method
cpg	348.54	J/molxK	583.71	Joback Method
cpg	361.71	J/molxK	618.83	Joback Method
cpg	374.11	J/molxK	653.94	Joback Method
cpg	385.75	J/molxK	689.06	Joback Method
cpg	396.66	J/molxK	724.18	Joback Method
cpg	406.85	J/molxK	759.30	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16518642&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16518642&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

# Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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

Latest version available from:

<https://www.chemeo.com/cid/14-793-6/3-CH3-2NC6H4COOCH3.pdf>

Generated by Cheméo on 2024-04-27 16:08:42.587036393 +0000 UTC m=+16523371.507613705.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.