

# 2,4-Dimethoxyamphetamine

<b>Other names:</b>	Benzeneethanamine,2,4-dimethoxy-«alpha»-methyl
<b>Inchi:</b>	InChI=1S/C11H17NO2/c1-8(12)6-9-4-5-10(13-2)7-11(9)14-3/h4-5,7-8H,6,12H2,1-3H3
<b>InchiKey:</b>	DQWOZMUBHQPF-UFHFFFAOYSA-N
<b>Formula:</b>	C11H17NO2
<b>SMILES:</b>	COc1ccc(CC(C)N)c(OC)c1
<b>Mol. weight [g/mol]:</b>	195.26
<b>CAS:</b>	23690-13-3

## Physical Properties

Property code	Value	Unit	Source
gf	-11.10	kJ/mol	Joback Method
hf	-292.71	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
ie	7.40	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	604.65	K	Joback Method
tc	818.55	K	Joback Method
tf	377.91	K	Joback Method
vc	0.603	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.34	J/molxK	604.65	Joback Method
cpg	428.28	J/molxK	640.30	Joback Method
cpg	442.45	J/molxK	675.95	Joback Method
cpg	455.85	J/molxK	711.60	Joback Method
cpg	468.48	J/molxK	747.25	Joback Method
cpg	480.33	J/molxK	782.90	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23690133&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23690133&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>ie:</b>	Ionization energy
<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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