

# Benzoic acid 4,5-dimethoxy-2-methoxy methyl-tetrahydro-pyran-3-yl ester

Inchi:	InChI=1S/C16H22O6/c1-18-9-11-7-14(19-2)15(20-3)8-13(11)16(17)22-12-5-4-6-21-10-12
InchiKey:	ZSWIENPEDRKNNH-UHFFFAOYSA-N
Formula:	C16H22O6
SMILES:	<chem>COCc1cc(OC)c(OC)cc1C(=O)OC1CCCOC1</chem>
Mol. weight [g/mol]:	310.34

## Physical Properties

Property code	Value	Unit	Source
gf	-443.23	kJ/mol	Joback Method
hf	-890.59	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.186		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2073.71		NIST Webbook
rinpol	2034.39		NIST Webbook
tb	797.15	K	Joback Method
tc	1016.48	K	Joback Method
tf	506.86	K	Joback Method
vc	0.856	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.15	J/molxK	797.15	Joback Method
cpg	779.49	J/molxK	979.92	Joback Method
cpg	768.74	J/molxK	943.37	Joback Method
cpg	756.50	J/molxK	906.81	Joback Method
cpg	742.81	J/molxK	870.26	Joback Method
cpg	727.68	J/molxK	833.70	Joback Method
cpg	788.72	J/molxK	1016.48	Joback Method
dvisc	0.0000515	Paxs	797.15	Joback Method

dvisc	0.0000645	Paxs	748.77	Joback Method
dvisc	0.0000834	Paxs	700.39	Joback Method
dvisc	0.0001120	Paxs	652.00	Joback Method
dvisc	0.0001577	Paxs	603.62	Joback Method
dvisc	0.0002356	Paxs	555.24	Joback Method
dvisc	0.0003801	Paxs	506.86	Joback Method

## Sources

<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=R273724&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R273724&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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