

# Meso-butanedioic acid, 2,3-dimethoxy-, dimethyl ester

Inchi:	InChI=1S/C8H14O6/c1-5(9)13-3-7(11)8(12)4-14-6(2)10/h7-8,11-12H,3-4H2,1-2H3
InchiKey:	PRZCCBBELKMZDR-UHFFFAOYSA-N
Formula:	C8H14O6
SMILES:	CC(=O)OCC(O)C(O)COC(C)=O
Mol. weight [g/mol]:	206.19
CAS:	53431-90-6

## Physical Properties

Property code	Value	Unit	Source
chs	-3958.00	kJ/mol	NIST Webbook
gf	-729.88	kJ/mol	Joback Method
hf	-1013.07	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	0.35		Crippen Method
logp	-1.166		Crippen Method
mcvol	150.200	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	718.50	K	Joback Method
tc	897.05	K	Joback Method
tf	415.88	K	Joback Method
vc	0.557	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.19	J/molxK	718.50	Joback Method
cpg	460.80	J/molxK	867.29	Joback Method
cpg	453.87	J/molxK	837.54	Joback Method
cpg	446.44	J/molxK	807.78	Joback Method
cpg	438.51	J/molxK	778.02	Joback Method
cpg	430.10	J/molxK	748.26	Joback Method
cpg	467.22	J/molxK	897.05	Joback Method
dvisc	0.0000099	Paxs	718.50	Joback Method

dvisc	0.0000173	Paxs	668.06	Joback Method
dvisc	0.0000331	Paxs	617.63	Joback Method
dvisc	0.0000712	Paxs	567.19	Joback Method
dvisc	0.0001777	Paxs	516.75	Joback Method
dvisc	0.0005404	Paxs	466.32	Joback Method
dvisc	0.0021532	Paxs	415.88	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=C53431906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53431906&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>chs:</b>	Standard solid enthalpy of combustion
<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>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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