

# Methyl sorbate

<b>Other names:</b>	2,4-Hexadienoic acid, methyl ester, (E,E)- Sorbic acid, methyl ester, (E,E)- Methyl trans,trans-sorbate 2-trans-4-trans-Methyl sorbate Methyl (E,E)-sorbate Sorbic acid, methyl ester Methyl (2E,4E)-hexadienoate Methyl (2E,4E)-2,4-hexadienoate (E,E)-2,4-Hexadienoic acid methyl ester Methyl (E,E)-2,4-hexadienoate Methyl (E,E)-hexa-2,4-dienoate 2,4-Hexadienoic acid, methyl ester, (2E,4E)-
<b>Inchi:</b>	InChI=1S/C7H10O2/c1-3-4-5-6-7(8)9-2/h3-6H,1-2H3/b4-3+,6-5+
<b>InchiKey:</b>	KWKVAGQCDSHWFK-VNKDHWASSA-N
<b>Formula:</b>	C7H10O2
<b>SMILES:</b>	<chem>CC=CC=CC(=O)OC</chem>
<b>Mol. weight [g/mol]:</b>	126.15
<b>CAS:</b>	689-89-4

## Physical Properties

Property code	Value	Unit	Source
gf	-65.42	kJ/mol	Joback Method
hf	-198.17	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	40.25	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.292		Crippen Method
mcvol	108.330	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	998.00		NIST Webbook
ripol	1448.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1444.00		NIST Webbook
tb	453.20	K	NIST Webbook
tc	638.38	K	Joback Method
tf	230.65	K	Joback Method
vc	0.411	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.48	J/molxK	444.17	Joback Method
cpg	253.23	J/molxK	606.02	Joback Method
cpg	244.83	J/molxK	573.65	Joback Method
cpg	235.98	J/molxK	541.28	Joback Method
cpg	226.65	J/molxK	508.91	Joback Method
cpg	216.82	J/molxK	476.54	Joback Method
cpg	261.19	J/molxK	638.38	Joback Method
dvisc	0.0001838	Paxs	444.17	Joback Method
dvisc	0.0002368	Paxs	408.58	Joback Method
dvisc	0.0003200	Paxs	373.00	Joback Method
dvisc	0.0004609	Paxs	337.41	Joback Method
dvisc	0.0007235	Paxs	301.82	Joback Method
dvisc	0.0012812	Paxs	266.24	Joback Method
dvisc	0.0027062	Paxs	230.65	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.20	K	2.70	NIST Webbook

# Sources

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C689894&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# 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>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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