Methyl sorbate

Other names:	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)-
Inchi:	InChI=1S/C7H10O2/c1-3-4-5-6-7(8)9-2/h3-6H,1-2H3/b4-3+,6-5+
InchiKey:	KWKVAGQCDSHWFK-VNKDHWASSA-N
Formula:	C7H10O2
SMILES:	CC=CC=CC(=O)OC
Mol. weight [g/mol]:	126.15
CAS:	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	1438.00		NIST Webbook
ripol	1448.00		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	m3/kmol	Joback Method

Temperature Dependent Properties

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

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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume