2,4-Hexadienedioic acid, dimethyl ester, (E,E)-

Other names:	trans,trans-Dimethyl muconate
	Dimethyl trans,trans-muconate
	Dimethyl (E,E)-muconate
Inchi:	InChI=1S/C8H10O4/c1-11-7(9)5-3-4-6-8(10)12-2/h3-6H,1-2H3/b5-3+,6-4+
InchiKey:	PXYBXMZVYNWQAM-GGWOSOGESA-N
Formula:	C8H10O4
SMILES:	COC(=O)C=CC=CC(=O)OC
Mol. weight [g/mol]:	170.16
CAS:	1119-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-290.92	kJ/mol	Joback Method
hf	-463.61	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	51.63	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.445		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	543.34	K	Joback Method
tc	743.39	K	Joback Method
tf	428.15 ± 5.00	K	NIST Webbook
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.47	J/mol×K	543.34	Joback Method
cpg	294.86	J/mol×K	576.68	Joback Method
cpg	304.73	J/mol×K	610.02	Joback Method
cpg	314.11	J/mol×K	643.36	Joback Method
cpg	322.99	J/mol×K	676.70	Joback Method
cpg	331.39	J/mol×K	710.05	Joback Method

cpg	339.32	J/mol×K	743.39	Joback Method
dvisc	0.0017248	Pa×s	314.08	Joback Method
dvisc	0.0009416	Pa×s	352.29	Joback Method
dvisc	0.0005787	Pa×s	390.50	Joback Method
dvisc	0.0003879	Pa×s	428.71	Joback Method
dvisc	0.0002776	Pa×s	466.92	Joback Method
dvisc	0.0002090	Pa×s	505.13	Joback Method
dvisc	0.0001637	Pa×s	543.34	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C1119433&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume