

3-Methyl-oct-2-enedioic acid dimethyl ester, E

Inchi:	InChI=1S/C10H16O4/c1-13-9(11)7-5-3-4-6-8-10(12)14-2/h5,7H,3-4,6,8H2,1-2H3/b7-5+
InchiKey:	RXTQXZGGNMYXAQ-FNORWQNLSA-N
Formula:	C10H16O4
SMILES:	COC(=O)C=CCCCC(=O)OC
Mol. weight [g/mol]:	200.23

Physical Properties

Property code	Value	Unit	Source
gf	-354.30	kJ/mol	Joback Method
hf	-622.11	kJ/mol	Joback Method
hfus	27.43	kJ/mol	Joback Method
hvap	56.12	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.449		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1530.00		NIST Webbook
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tb	584.94	K	Joback Method
tc	772.08	K	Joback Method
tf	341.70	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.88	J/mol×K	584.94	Joback Method
cpg	408.59	J/mol×K	616.13	Joback Method
cpg	420.72	J/mol×K	647.32	Joback Method
cpg	432.29	J/mol×K	678.51	Joback Method
cpg	443.29	J/mol×K	709.70	Joback Method
cpg	453.74	J/mol×K	740.89	Joback Method
cpg	463.64	J/mol×K	772.08	Joback Method
dvisc	0.0017602	Pa×s	341.70	Joback Method

dvisc	0.0009565	Pa×s	382.24	Joback Method
dvisc	0.0005843	Pa×s	422.78	Joback Method
dvisc	0.0003891	Pa×s	463.32	Joback Method
dvisc	0.0002766	Pa×s	503.86	Joback Method
dvisc	0.0002069	Pa×s	544.40	Joback Method
dvisc	0.0001611	Pa×s	584.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249360&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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