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

Inchi: InChI=1S/C7H10O4/c1-11-7(10)5-3-2-4-6(8)9/h2,4H,3,5H2,1H3,(H,8,9)/b4-2+
InchiKey: HBZOSRCVWPAGOA-DUXPYHPUSA-N
Formula: C7H10O4
SMILES: COC(=O)CCC=CC(=O)O
Mol. weight [g/mol]: 158.15

Physical Properties

Property code	Value	Unit	Source
gf	-411.38	kJ/mol	Joback Method
hf	-580.20	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.580		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1287.00		NIST Webbook
tb	586.06	K	Joback Method
tc	770.92	K	Joback Method
tf	346.48	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.10	J/mol×K	586.06	Joback Method
cpg	290.62	J/mol×K	616.87	Joback Method
cpg	298.72	J/mol×K	647.68	Joback Method
cpg	306.42	J/mol×K	678.49	Joback Method
cpg	313.73	J/mol×K	709.30	Joback Method
cpg	320.65	J/mol×K	740.11	Joback Method
cpg	327.20	J/mol×K	770.92	Joback Method
dvisc	0.0044440	Pa×s	346.48	Joback Method
dvisc	0.0016709	Pa×s	386.41	Joback Method

dvisc	0.0007546	Pa×s	426.34	Joback Method
dvisc	0.0003905	Pa×s	466.27	Joback Method
dvisc	0.0002242	Pa×s	506.20	Joback Method
dvisc	0.0001396	Pa×s	546.13	Joback Method
dvisc	0.0000927	Pa×s	586.06	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=R249320&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume