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

Inchi: InChI=1S/C11H18O4/c1-14-10(12)8-6-4-3-5-7-9-11(13)15-2/h6,8H,3-5,7,9H2,1-2H3/b8-6
InchiKey: AYRXFAMQOIQKRZ-SOFGYWHQSA-N
Formula: C11H18O4
SMILES: COC(=O)C=CCCCCCC(=O)OC
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	-345.88	kJ/mol	Joback Method
hf	-642.75	kJ/mol	Joback Method
hfus	30.02	kJ/mol	Joback Method
hvap	58.35	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.839		Crippen Method
mcvol	176.430	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1621.00		NIST Webbook
tb	607.82	K	Joback Method
tc	793.03	K	Joback Method
tf	352.97	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.66	J/mol×K	607.82	Joback Method
cpg	458.09	J/mol×K	638.69	Joback Method
cpg	470.91	J/mol×K	669.56	Joback Method
cpg	483.11	J/mol×K	700.43	Joback Method
cpg	494.71	J/mol×K	731.29	Joback Method
cpg	505.71	J/mol×K	762.16	Joback Method
cpg	516.13	J/mol×K	793.03	Joback Method
dvisc	0.0016775	Pa×s	352.97	Joback Method
dvisc	0.0008965	Pa×s	395.44	Joback Method

dvisc	0.0005410	Pa×s	437.92	Joback Method
dvisc	0.0003570	Pa×s	480.39	Joback Method
dvisc	0.0002520	Pa×s	522.87	Joback Method
dvisc	0.0001875	Pa×s	565.35	Joback Method
dvisc	0.0001454	Pa×s	607.82	Joback Method

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=R249340&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume