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

Inchi: InChI=1S/C9H14O4/c1-7(6-9(11)13-3)4-5-8(10)12-2/h6H,4-5H2,1-3H3/b7-6-
InchiKey: TZZBSTDITUFGQX-SREVYHEPSA-N
Formula: C9H14O4
SMILES: COC(=O)C=C(C)CCC(=O)OC
Mol. weight [g/mol]: 186.21

Physical Properties

Property code	Value	Unit	Source
gf	-371.27	kJ/mol	Joback Method
hf	-611.26	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.059		Crippen Method
mcvol	148.250	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1278.00		NIST Webbook
tb	561.94	K	Joback Method
tc	754.41	K	Joback Method
tf	316.47	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.59	J/mol×K	561.94	Joback Method
cpg	360.64	J/mol×K	594.02	Joback Method
cpg	372.16	J/mol×K	626.10	Joback Method
cpg	383.14	J/mol×K	658.17	Joback Method
cpg	393.58	J/mol×K	690.25	Joback Method
cpg	403.50	J/mol×K	722.33	Joback Method
cpg	412.90	J/mol×K	754.41	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=R249335&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
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