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

Inchi: InChI=1S/C10H16O4/c1-8(7-10(12)14-3)5-4-6-9(11)13-2/h7H,4-6H2,1-3H3/b8-7-

InchiKey: TWMLHHSLTDYVBK-FPLPWBNLSA-N

Formula: C10H16O4

SMILES: COC(=O)C=C(C)CCCC(=O)OC

Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
gf	-362.85	kJ/mol	Joback Method
hf	-631.90	kJ/mol	Joback Method
hfus	26.12	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.449		Crippen Method
mcvol	162.340	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1373.00		NIST Webbook
tb	584.82	K	Joback Method
tc	774.95	K	Joback Method
tf	327.74	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.67	J/mol×K	584.82	Joback Method
cpg	408.54	J/mol×K	616.51	Joback Method
cpg	420.83	J/mol×K	648.20	Joback Method
cpg	432.54	J/mol×K	679.88	Joback Method
cpg	443.67	J/mol×K	711.57	Joback Method
cpg	454.23	J/mol×K	743.26	Joback Method
cpg	464.22	J/mol×K	774.95	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=R249315&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