2-Methyl-but-2-enedioic acid dimethyl ester

Other names: Dimethyl mesaconate
Inchi: InChI=1S/C7H10O4/c1-5(7(9)11-3)4-6(8)10-2/h4H,1-3H3/b5-4+
InchiKey: WQEXBUQDXKPVHR-SNAWJCMRSA-N
Formula: C7H10O4
SMILES: COC(=O)C=C(C)C(=O)OC
Mol. weight [g/mol]: 158.15
CAS: 617-53-8

Physical Properties

Property code	Value	Unit	Source
gf	-388.11	kJ/mol	Joback Method
hf	-569.98	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	49.53	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.279		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1055.00		NIST Webbook
tb	516.18	K	Joback Method
tc	713.77	K	Joback Method
tf	293.93	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.95	J/mol×K	680.84	Joback Method
cpg	259.92	J/mol×K	516.18	Joback Method
cpg	269.97	J/mol×K	549.11	Joback Method
cpg	279.60	J/mol×K	582.04	Joback Method
cpg	288.81	J/mol×K	614.98	Joback Method
cpg	297.60	J/mol×K	647.91	Joback Method
cpg	313.89	J/mol×K	713.77	Joback Method

hvapt	55.20	kJ/mol	399.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617538&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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