Butanedioic acid, methylene-, dimethyl ester

Other names:	Succinic acid, methylene-, dimethyl ester
	Dimethyl itaconate
	Itaconic acid, dimethyl ester
	Methylenesuccinic acid, dimethyl ester
	Dimethyl methylenesuccinate
	Butanedioic acid, 2-methylene-, dimethyl ester
	Dimethyl 2-methylenesuccinate
Inchi:	InChI=1S/C7H10O4/c1-5(7(9)11-3)4-6(8)10-2/h1,4H2,2-3H3
InchiKey:	ZWWQRMFIZFPUAA-UHFFFAOYSA-N
Formula:	C7H10O4
SMILES:	C=C(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	158.15
CAS:	617-52-7

Physical Properties

Property code	Value	Unit	Source
gf	-380.49	kJ/mol	Joback Method
hf	-561.77	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.279		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1096.50		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1059.00		NIST Webbook
tb	481.20	K	NIST Webbook
tc	701.54	K	Joback Method
tf	297.25	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.22	J/mol×K	508.70	Joback Method
cpg	270.10	J/mol×K	540.84	Joback Method
cpg	279.61	J/mol×K	572.98	Joback Method
cpg	288.73	J/mol×K	605.12	Joback Method
cpg	297.46	J/mol×K	637.26	Joback Method
cpg	305.79	J/mol×K	669.40	Joback Method
cpg	313.72	J/mol×K	701.54	Joback Method
hvapt	67.00	kJ/mol	411.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	1.50	NIST Webbook

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=C617527&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume