cis-2-Methyl-2-butenedioic acid, dimethyl ester

Other names:	Citraconic acid, dimethyl ester
	Dimethyl citraconate
	Dimethyl methyl maleate
	Methylmaleic acid, dimethyl ester
	2-Butenedioic acid, 2-methyl-, dimethyl ester (Z)-
	Maleic acid, methyl-, dimethyl ester
	2-Methyl-but-2-enedioic acid dimethyl ester, Z
Inchi:	InChI=1S/C7H10O4/c1-5(7(9)11-3)4-6(8)10-2/h4H,1-3H3/b5-4-
InchiKey:	WQEXBUQDXKPVHR-PLNGDYQASA-N
Formula:	C7H10O4
SMILES:	COC(=O)C=C(C)C(=O)OC
Mol. weight [g/mol]:	158.15
CAS:	617-54-9

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	1058.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1056.00		NIST Webbook
tb	483.70	K	NIST Webbook
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	55.80	kJ/mol	404.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.00	K	1.30	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C617549&Units=SI

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