Butanedioic acid, methoxy-, dimethyl ester

Other names:	Succinic acid, methoxy-, dimethyl ester
	Dimethyl methoxybutane-1,4-dioate
	DL-Malic acid, methyl ether, dimethyl ester
	2-Methoxy-succinic acid dimethyl ester
Inchi:	InChI=1S/C7H12O5/c1-10-5(7(9)12-3)4-6(8)11-2/h5H,4H2,1-3H3
InchiKey:	CZGCYHISZCRQFR-UHFFFAOYSA-N
Formula:	C7H12O5
SMILES:	COC(=O)CC(OC)C(=O)OC
Mol. weight [g/mol]:	176.17
CAS:	4148-97-4

Physical Properties

Property code	Value	Unit	Source
gf	-567.22	kJ/mol	Joback Method
hf	-814.91	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	0.32		Crippen Method
logp	-0.263		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1146.10		NIST Webbook
rinpol	1113.00		NIST Webbook
tb	534.12	K	Joback Method
tc	722.52	K	Joback Method
tf	320.20	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.30	J/mol×K	534.12	Joback Method
cpg	311.97	J/mol×K	565.52	Joback Method

cpg	322.29	J/mol×K	596.92	Joback Method
cpg	332.23	J/mol×K	628.32	Joback Method
cpg	341.79	J/mol×K	659.72	Joback Method
cpg	350.93	J/mol×K	691.12	Joback Method
cpg	359.64	J/mol×K	722.52	Joback Method
dvisc	0.0019697	Pa×s	320.20	Joback Method
dvisc	0.0010986	Pa×s	355.85	Joback Method
dvisc	0.0006815	Pa×s	391.51	Joback Method
dvisc	0.0004578	Pa×s	427.16	Joback Method
dvisc	0.0003270	Pa×s	462.81	Joback Method
dvisc	0.0002451	Pa×s	498.47	Joback Method
dvisc	0.0001909	Pa×s	534.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4148974&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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