Butanedioic acid, monomethyl ester

Other names:	Succinic acid, monomethyl ester
	Methyl hydrogen succinate
	Monomethyl succinate
	3-Carbomethoxypropanoic acid
Inchi:	InChI=1S/C5H8O4/c1-9-5(8)3-2-4(6)7/h2-3H2,1H3,(H,6,7)
InchiKey:	JDRMYOQETPMYQX-UHFFFAOYSA-N
Formula:	C5H8O4
SMILES:	COC(=O)CCC(=O)O
Mol. weight [g/mol]:	132.11
CAS:	3878-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-508.44	kJ/mol	Joback Method
hf	-656.14	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	59.30	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	0.024		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
rinpol	1106.10		NIST Webbook
tb	536.14	K	Joback Method
tc	717.47	K	Joback Method
tf	329.02	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.18	J/mol×K	536.14	Joback Method
cpg	222.33	J/mol×K	566.36	Joback Method
cpg	229.20	J/mol×K	596.58	Joback Method
cpg	235.78	J/mol×K	626.80	Joback Method

cpg	242.07	J/mol×K	657.02	Joback Method
cpg	248.07	J/mol×K	687.25	Joback Method
cpg	253.78	J/mol×K	717.47	Joback Method
dvisc	0.0060367	Pa×s	329.02	Joback Method
dvisc	0.0024566	Pa×s	363.54	Joback Method
dvisc	0.0011684	Pa×s	398.06	Joback Method
dvisc	0.0006257	Pa×s	432.58	Joback Method
dvisc	0.0003675	Pa×s	467.10	Joback Method
dvisc	0.0002322	Pa×s	501.62	Joback Method
dvisc	0.0001557	Pa×s	536.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.20	K	2.70	NIST Webbook
tbrp	395.20	K	0.50	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=C3878555&Units=SI

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