Propanedioic acid, ethyl-, dimethyl ester

Other names:	Malonic acid, ethyl-, dimethyl ester
	Dimethyl ethylmalonate
	2-Ethyl-malonic acid dimethyl ester
Inchi:	InChI=1S/C7H12O4/c1-4-5(6(8)10-2)7(9)11-3/h5H,4H2,1-3H3
InchiKey:	XGRMVENQJLQMLT-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CCC(C(=O)OC)C(=O)OC
Mol. weight [g/mol]:	160.17
CAS:	26717-67-9

Physical Properties

Property code	Value	Unit	Source
gf	-462.22	kJ/mol	Joback Method
hf	-682.69	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.359		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1011.00		NIST Webbook
rinpol	1011.00		NIST Webbook
tb	511.70	K	Joback Method
tc	701.34	K	Joback Method
tf	297.97	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.59	J/mol×K	511.70	Joback Method
cpg	289.32	J/mol×K	543.31	Joback Method
cpg	299.65	J/mol×K	574.91	Joback Method
cpg	309.59	J/mol×K	606.52	Joback Method

cpg	319.13	J/mol×K	638.13	Joback Method
cpg	328.25	J/mol×K	669.73	Joback Method
cpg	336.95	J/mol×K	701.34	Joback Method
dvisc	0.0027013	Pa×s	297.97	Joback Method
dvisc	0.0014459	Pa×s	333.59	Joback Method
dvisc	0.0008732	Pa×s	369.21	Joback Method
dvisc	0.0005762	Pa×s	404.84	Joback Method
dvisc	0.0004067	Pa×s	440.46	Joback Method
dvisc	0.0003024	Pa×s	476.08	Joback Method
dvisc	0.0002344	Pa×s	511.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26717679&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

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