2-Pentenedioic acid, dimethyl ester

Other names:	Glutaconic acid, dimethyl ester
	Dimethyl glutaconate
Inchi:	InChI=1S/C7H10O4/c1-10-6(8)4-3-5-7(9)11-2/h3-4H,5H2,1-2H3/b4-3+
InchiKey:	SKCGFFOFYXLNCG-ONEGZZNKSA-N
Formula:	C7H10O4
SMILES:	COC(=O)C=CCC(=O)OC
Mol. weight [g/mol]:	158.15
CAS:	5164-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-379.56	kJ/mol	Joback Method
hf	-560.19	kJ/mol	Joback Method
hfus	19.66	kJ/mol	Joback Method
hvap	49.45	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.279		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1187.00		NIST Webbook
tb	516.30	K	Joback Method
tc	710.37	K	Joback Method
tf	307.89	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.06	J/mol×K	516.30	Joback Method
cpg	269.96	J/mol×K	548.64	Joback Method
cpg	279.46	J/mol×K	580.99	Joback Method
cpg	288.55	J/mol×K	613.33	Joback Method
cpg	297.23	J/mol×K	645.68	Joback Method
cpg	305.50	J/mol×K	678.02	Joback Method

cpg	313.35	J/mol×K	710.37	Joback Method
dvisc	0.0018974	Pa×s	307.89	Joback Method
dvisc	0.0010904	Pa×s	342.62	Joback Method
dvisc	0.0006939	Pa×s	377.36	Joback Method
dvisc	0.0004765	Pa×s	412.09	Joback Method
dvisc	0.0003469	Pa×s	446.83	Joback Method
dvisc	0.0002644	Pa×s	481.56	Joback Method
dvisc	0.0002090	Pa×s	516.30	Joback Method

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=C5164761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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