PROPANEDIOIC ACID, METHYL-, DIMETHYL ESTER

Other names: Malonic acid, methyl-, dimethyl ester
Dimethyl methylmalonate
Propanedioic acid, 2-methyl-, dimethyl ester
Maleic acid, dimethyl ester

Inchi: InChI=1S/C6H10O4/c1-4(5(7)9-2)6(8)10-3/h4H,1-3H3

InchiKey: LRBPFPZTIZSOGG-UHFFFAOYSA-N

Formula: C6H10O4

SMILES: COC(=O)C(C)C(=O)OC

Mol. weight [g/mol]: 146.14

Physical Properties

Property code	Value	Unit	Source
af	0.4650		Cheméo Relay (1.0)
chl	-2963.90 ± 0.54	kJ/mol	NIST Webbook
hf	-768.56 ± 0.88	kJ/mol	NIST Webbook
hfl	-826.34 ± 0.54	kJ/mol	NIST Webbook
hfus	13.35	kJ/mol	Joback Method
hvap	57.78 ± 0.71	kJ/mol	NIST Webbook
hvap	57.80	kJ/mol	NIST Webbook
ie	10.21	eV	Cheméo Relay (1.0)
log10ws	-0.46		Cheméo Relay (1.0)
logp	-0.031		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	960.70		NIST Webbook
rinpol	960.70		NIST Webbook
tb	449.70	K	NIST Webbook
tc	610.43	K	Cheméo Relay (1.0)
tf	250.96	K	Cheméo Relay (1.0)
vc	0.408	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	289.02	J/mol×K	680.73	Joback Method
cpg	236.68	J/mol×K	488.82	Joback Method
cpg	246.23	J/mol×K	520.80	Joback Method
cpg	255.46	J/mol×K	552.79	Joback Method
cpg	264.37	J/mol×K	584.77	Joback Method
cpg	281.17	J/mol×K	648.74	Joback Method
cpg	272.95	J/mol×K	616.76	Joback Method
cpl	261.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0027257	Pa×s	286.70	Joback Method
dvisc	0.0014884	Pa×s	320.39	Joback Method
dvisc	0.0009119	Pa×s	354.07	Joback Method
dvisc	0.0006083	Pa×s	387.76	Joback Method
dvisc	0.0004330	Pa×s	421.45	Joback Method
dvisc	0.0003241	Pa×s	455.13	Joback Method
dvisc	0.0002524	Pa×s	488.82	Joback Method
hvapt	57.80 ± 0.80	kJ/mol	293.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C609029&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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
ie:	Ionization energy
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