BUTANOIC ACID, 4-METHOXY-3-OXO-, METHYL ESTER

Other names: Butanoic acid, 4-methoxy-3-oxo-, methyl ester
Methyl methoxyacetoacetate
methyl 4-methoxy-3-oxobutyrate

Inchi: InChI=1S/C6H10O4/c1-9-4-5(7)3-6(8)10-2/h3-4H2,1-2H3

InchiKey: QGBPKJFJAVDUNC-UHFFFAOYSA-N

Formula: C6H10O4

SMILES: COCC(=O)CC(=O)OC

Mol. weight [g/mol]: 146.14

Physical Properties

Property code	Value	Unit	Source
af	0.5092		Cheméo Relay (1.0)
hf	-700.22	kJ/mol	Cheméo Relay (1.0)
hfus	16.87	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-3.48e-03		Cheméo Relay (1.0)
logp	-0.235		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	469.00	K	Cheméo Relay (1.0)
tc	648.44	K	Cheméo Relay (1.0)
tf	279.62	K	Cheméo Relay (1.0)
vc	0.396	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.42	J/mol×K	489.26	Joback Method
cpg	245.69	J/mol×K	520.56	Joback Method
cpg	254.67	J/mol×K	551.86	Joback Method
cpg	263.35	J/mol×K	583.16	Joback Method
cpg	271.71	J/mol×K	614.46	Joback Method
cpg	279.74	J/mol×K	645.76	Joback Method

cpg	287.43	J/mol×K	677.07	Joback Method
dvisc	0.0020653	Pa×s	301.70	Joback Method
dvisc	0.0012506	Pa×s	332.96	Joback Method
dvisc	0.0008254	Pa×s	364.22	Joback Method
dvisc	0.0005818	Pa×s	395.48	Joback Method
dvisc	0.0004316	Pa×s	426.74	Joback Method
dvisc	0.0003335	Pa×s	458.00	Joback Method
dvisc	0.0002663	Pa×s	489.26	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41051154&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
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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