Dimethyl (2e)-2-butenedioate

Inchi: InChI=1S/C6H8O4/c1-9-5(7)3-4-6(8)10-2/h3-4H,1-2H3
InchiKey: LDCRTTXIJACKKU-ONEGZZNKSA-N
Formula: C6H8O4
SMILES: COC(=O)/C=C/C(=O)OC
Mol. weight [g/mol]: 144.13

Physical Properties

Property code	Value	Unit	Source
af	0.5135		Cheméo Relay (1.0)
hf	-689.25	kJ/mol	Cheméo Relay (1.0)
hfus	17.07	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Cheméo Relay (1.0)
ie	10.58	eV	Cheméo Relay (1.0)
log10ws	-1.93		Cheméo Relay (1.0)
logp	-0.111		Crippen Method
mcvol	105.980	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	474.03	K	Cheméo Relay (1.0)
tc	628.40	K	Cheméo Relay (1.0)
tf	370.35	K	Cheméo Relay (1.0)
vc	0.388	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.65	J/mol×K	493.42	Joback Method
cpg	265.80	J/mol×K	689.99	Joback Method
cpg	258.82	J/mol×K	657.23	Joback Method
cpg	251.49	J/mol×K	624.47	Joback Method
cpg	243.80	J/mol×K	591.71	Joback Method
cpg	235.76	J/mol×K	558.94	Joback Method
cpg	227.37	J/mol×K	526.18	Joback Method
dvisc	0.0004981	Pa×s	395.02	Joback Method
dvisc	0.0002234	Pa×s	493.42	Joback Method

dvisc	0.0002809	Pa×s	460.62	Joback Method
dvisc	0.0003660	Pa×s	427.82	Joback Method
dvisc	0.0018904	Pa×s	296.62	Joback Method
dvisc	0.0007168	Pa×s	362.22	Joback Method
dvisc	0.0011092	Pa×s	329.42	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009491&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

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