2-Butynedioic acid, dimethyl ester

Other names:	Acetylenedicarboxylic acid, dimethyl ester
	Bis(methoxycarbonyl)acetylene
	Dimethyl acetylenedicarboxylate
	Dimethyl butynedioate
	Dimethyl 2-butynedioate
	Methyl acetylenedicarboxylate
	1,2-Bis(methoxycarbonyl)acetylene
	Dimethyl acetylenedicarboxylic acid
	Dimethyl 1,2-acetylenedicarboxylate
	Dimethyl butyne-1,4-dioate
	Dimethyl ethynedicarboxylate
	1,2-Bis(methoxycarbonyl)ethyne
	Butynedioic acid dimethyl ester
	Bis(carbomethoxy)acetylene
	Di(carbomethoxy)acetylene
	But-2-ynedioic acid dimethyl ester
	2-Butynedioic acid, 1,4-dimethyl ester
	NSC 14912
Inchi:	InChI=1S/C6H6O4/c1-9-5(7)3-4-6(8)10-2/h1-2H3
InchiKey:	VHILMKFSCRWWIJ-UHFFFAOYSA-N
Formula:	C6H6O4
SMILES:	COC(=O)C#CC(=O)OC
Mol. weight [g/mol]:	142.11
CAS:	762-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-265.40	kJ/mol	Joback Method
hf	-384.47	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	49.41	kJ/mol	Joback Method
ie	10.90	eV	NIST Webbook
log10ws	0.15		Crippen Method
logp	-0.664		Crippen Method
mcvol	101.680	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	498.26	K	Joback Method

tc	711.06	K	Joback Method
tf	407.80	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.31	J/mol×K	498.26	Joback Method
cpg	210.17	J/mol×K	533.73	Joback Method
cpg	217.79	J/mol×K	569.19	Joback Method
cpg	225.15	J/mol×K	604.66	Joback Method
cpg	232.23	J/mol×K	640.13	Joback Method
cpg	239.01	J/mol×K	675.59	Joback Method
cpg	245.46	J/mol×K	711.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.70	K	2.50	NIST Webbook

Sources

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=C762425&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume