2-Butynedioic acid, diethyl ester

Other names:	Acetylenedicarboxylic acid, diethyl ester
	Bis-(Ethoxycarbonyl)acetylene
	Di-Ethyl acetylenedicarboxylate
	diethyl 2-butynedioate
Inchi:	InChI=1S/C8H10O4/c1-3-11-7(9)5-6-8(10)12-4-2/h3-4H2,1-2H3
InchiKey:	STRNXFOUBFLVIN-UHFFFAOYSA-N
Formula:	C8H10O4
SMILES:	CCOC(=O)C#CC(=O)OCC
Mol. weight [g/mol]:	170.16
CAS:	762-21-0

Physical Properties

Property code	Value	Unit	Source
chl	-4010.00	kJ/mol	NIST Webbook
gf	-248.56	kJ/mol	Joback Method
hf	-425.75	kJ/mol	Joback Method
hfl	-567.20 ± 4.00	kJ/mol	NIST Webbook
hfl	600.80	kJ/mol	NIST Webbook
hfus	25.17	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.116		Crippen Method
mcvol	129.860	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	544.02	K	Joback Method
tc	750.31	K	Joback Method
tf	430.34	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.58	J/mol×K	544.02	Joback Method
cpg	296.01	J/mol×K	578.40	Joback Method

cpg	306.03	J/mol×K	612.78	Joback Method
cpg	315.63	J/mol×K	647.17	Joback Method
cpg	324.79	J/mol×K	681.55	Joback Method
cpg	333.49	J/mol×K	715.93	Joback Method
cpg	341.73	J/mol×K	750.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.70	K	1.50	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=C762210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
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
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