2-Propynoic acid, methyl ester

Other names:	Propiolic acid, methyl ester
	Methyl acetylenecarboxylate
	Methyl ethynecarboxylate
	Methyl propiolate
	Methyl propynoate
	Acetylenecarboxylic acid methyl ester
	Propynoic acid, methyl ester
	NSC 154164
Inchi:	InChI=1S/C4H4O2/c1-3-4(5)6-2/h1H,2H3
InchiKey:	IMAKHNTVDGLIRY-UHFFFAOYSA-N
Formula:	C4H4O2
SMILES:	C#CC(=O)OC
Mol. weight [g/mol]:	84.07
CAS:	922-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-28.05	kJ/mol	Joback Method
hf	-78.79	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	36.30 ± 0.30	kJ/mol	NIST Webbook
hvap	35.60 ± 0.40	kJ/mol	NIST Webbook
hvap	28.90	kJ/mol	NIST Webbook
hvap	35.80 ± 0.10	kJ/mol	NIST Webbook
hvap	35.90 ± 0.10	kJ/mol	NIST Webbook
ie	10.75	eV	NIST Webbook
ie	10.30	eV	NIST Webbook
log10ws	-0.15		Crippen Method
logp	-0.207		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
pc	5044.23	kPa	Joback Method
tb	377.00 ± 1.00	K	NIST Webbook
tb	377.20	K	NIST Webbook
tc	550.07	K	Joback Method
tf	253.97	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.53	J/mol×K	550.07	Joback Method
cpg	131.45	J/mol×K	517.95	Joback Method
cpg	127.23	J/mol×K	485.82	Joback Method
cpg	122.85	J/mol×K	453.70	Joback Method
cpg	118.32	J/mol×K	421.58	Joback Method
cpg	113.64	J/mol×K	389.45	Joback Method
cpg	108.82	J/mol×K	357.33	Joback Method
hvapt	31.50 ± 0.10	kJ/mol	363.00	NIST Webbook
hvapt	32.10 ± 0.10	kJ/mol	355.00	NIST Webbook
hvapt	32.80 ± 0.10	kJ/mol	344.00	NIST Webbook
hvapt	33.80 ± 0.10	kJ/mol	331.00	NIST Webbook
hvapt	34.20 ± 0.10	kJ/mol	326.00	NIST Webbook
hvapt	34.90 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	35.90	kJ/mol	323.00	NIST Webbook
hvapt	32.80	kJ/mol	419.50	NIST Webbook
hvapt	39.10	kJ/mol	292.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C922678&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume