Propiolic acid, 3-phenyl-, methyl ester

Other names:	2-Propynoic acid, 3-phenyl-, methyl ester
	Methyl 3-phenyl-2-propynoate
	Methyl 3-phenylpropiolate
	Methyl 3-phenylpropynoate
	Methyl phenylacetylenecarboxylate
	Methyl phenylethynecarboxylate
	Methyl phenylpropiolate
	Methyl phenylpropynoate
	Propiolic acid, phenyl-, methyl ester
	2-Phenyl-1-carbomethoxyacetylene
	Phenylpropynoic acid methyl ester
Inchi:	InChI=1S/C10H8O2/c1-12-10(11)8-7-9-5-3-2-4-6-9/h2-6H,1H3
InchiKey:	JFGWPXKGINUNDH-UHFFFAOYSA-N
Formula:	C10H8O2
SMILES:	COC(=O)C#Cc1ccccc1
Mol. weight [g/mol]:	160.17
CAS:	4891-38-7

Physical Properties

Property code	Value	Unit	Source
chl	-5009.90	kJ/mol	NIST Webbook
gf	114.61	kJ/mol	Joback Method
hf	14.30	kJ/mol	Joback Method
hfl	-68.50 ± 5.00	kJ/mol	NIST Webbook
hfl	99.60	kJ/mol	NIST Webbook
hfus	21.61	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.211		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	540.17	K	Joback Method
tc	781.41	K	Joback Method
tf	290.00 ± 1.00	K	NIST Webbook
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.21	J/mol×K	540.17	Joback Method
cpg	276.68	J/mol×K	580.38	Joback Method
cpg	288.37	J/mol×K	620.58	Joback Method
cpg	299.27	J/mol×K	660.79	Joback Method
cpg	309.43	J/mol×K	701.00	Joback Method
cpg	318.84	J/mol×K	741.20	Joback Method
cpg	327.54	J/mol×K	781.41	Joback Method

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=C4891387&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume