Ethylphenylpropiolate

Other names:	Ethyl 3-phenylpropiolate
	Ethyl phenylacetylenecarboxylate
	2-Propynoic acid, 3-phenyl-, ethyl ester
	Ethyl phenylpropriolate
	Phenylacetylene monocarboxylic acid ethyl ester
	Propiolic acid, phenyl-, ethyl ester
	Ethyl phenylpropynoate
	Ethyl 3-phenylpropynoate
	NSC 41566
	3-Phenyl-2-propynoic acid ethyl ester
	ethyl 3-phenylprop-2-ynoate
Inchi:	InChI=1S/C11H10O2/c1-2-13-11(12)9-8-10-6-4-3-5-7-10/h3-7H,2H2,1H3
InchiKey:	ACJOYTKWHPEIHW-UHFFFAOYSA-N
Formula:	C11H10O2
SMILES:	CCOC(=O)C#Cc1ccccc1
Mol. weight [g/mol]:	174.20
CAS:	2216-94-6

Physical Properties

Property code	Value	Unit	Source
chl	-5606.10	kJ/mol	NIST Webbook
gf	123.03	kJ/mol	Joback Method
hf	-6.34	kJ/mol	Joback Method
hfl	189.00	kJ/mol	NIST Webbook
hfl	-151.70 ± 5.00	kJ/mol	NIST Webbook
hfus	24.20	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.601		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	538.20	K	NIST Webbook
tb	538.00 ± 5.00	K	NIST Webbook
tc	799.43	K	Joback Method
tf	418.41	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.87	J/mol×K	563.05	Joback Method
cpg	322.37	J/mol×K	602.45	Joback Method
cpg	335.03	J/mol×K	641.84	Joback Method
cpg	346.86	J/mol×K	681.24	Joback Method
cpg	357.87	J/mol×K	720.64	Joback Method
cpg	368.10	J/mol×K	760.03	Joback Method
cpg	377.57	J/mol×K	799.43	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216946&Units=SI

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