

Ethyl propiolate

Other names:	Ethyl acetylenecarboxylate Propiolic acid ethyl ester Ethyl propynoate 2-Propynoic acid, ethyl ester (Ethoxycarbonyl)acetylene Ethyl 2-propynoate
Inchi:	InChI=1S/C5H6O2/c1-3-5(6)7-4-2/h1H,4H2,2H3
InchiKey:	FMVJYQGSRWVMQV-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	C#CC(=O)OCC
Mol. weight [g/mol]:	98.10
CAS:	623-47-2

Physical Properties

Property code	Value	Unit	Source
chl	-2659.00	kJ/mol	NIST Webbook
gf	-19.63	kJ/mol	Joback Method
hf	-99.43	kJ/mol	Joback Method
hfl	-166.00 ± 3.00	kJ/mol	NIST Webbook
hfl	187.00	kJ/mol	NIST Webbook
hfus	14.47	kJ/mol	Joback Method
hvap	35.74	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.183		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
tb	392.65 ± 2.00	K	NIST Webbook
tb	393.00	K	NIST Webbook
tb	393.20	K	NIST Webbook
tc	572.00	K	Joback Method
tf	265.24	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.27	J/mol×K	380.21	Joback Method
cpg	146.80	J/mol×K	412.17	Joback Method
cpg	153.11	J/mol×K	444.14	Joback Method
cpg	159.19	J/mol×K	476.10	Joback Method
cpg	165.05	J/mol×K	508.07	Joback Method
cpg	170.68	J/mol×K	540.03	Joback Method
cpg	176.08	J/mol×K	572.00	Joback Method

Sources

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=C623472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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