

Ethyl 2-butynoate

Other names:	Ethyl tetrolate 2-Butynoic acid, ethyl ester Tetrolic acid, ethyl ester Ethyl 1-propynecarboxylate Ethyl 3-methylpropiolate
Inchi:	InChI=1S/C6H8O2/c1-3-5-6(7)8-4-2/h4H2,1-2H3
InchiKey:	FCJJZKCJURDYNF-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	CC#CC(=O)OCC
Mol. weight [g/mol]:	112.13
CAS:	4341-76-8

Physical Properties

Property code	Value	Unit	Source
gf	-31.48	kJ/mol	Joback Method
hf	-139.67	kJ/mol	Joback Method
hfus	17.21	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.573		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	436.20	K	NIST Webbook
tc	625.16	K	Joback Method
tf	335.64	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.07	J/mol×K	421.97	Joback Method
cpg	180.45	J/mol×K	455.84	Joback Method
cpg	188.58	J/mol×K	489.70	Joback Method
cpg	196.44	J/mol×K	523.57	Joback Method

cpg	204.02	J/mol×K	557.43	Joback Method
cpg	211.32	J/mol×K	591.30	Joback Method
cpg	218.34	J/mol×K	625.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	25.30	NIST Webbook

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=C4341768&Units=SI

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
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

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