

Ethoxyacetylene

Other names:	Ethyl ethynyl ether Ethoxyethyne Ethyne, ethoxy- Ether, ethyl ethynyl
Inchi:	InChI=1S/C4H6O/c1-3-5-4-2/h1H,4H2,2H3
InchiKey:	WMYNMYVRWWCRPS-UHFFFAOYSA-N
Formula:	C4H6O
SMILES:	C#COCC
Mol. weight [g/mol]:	70.09
CAS:	927-80-0

Physical Properties

Property code	Value	Unit	Source
gf	100.87	kJ/mol	Joback Method
hf	33.79	kJ/mol	Joback Method
hfus	10.28	kJ/mol	Joback Method
hvap	26.77	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.614		Crippen Method
mcvol	64.490	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
rinpol	498.00		NIST Webbook
rinpol	498.00		NIST Webbook
tb	303.46	K	Joback Method
tc	478.93	K	Joback Method
tf	204.04	K	Joback Method
vc	0.239	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.08	J/mol×K	303.46	Joback Method
cpg	105.25	J/mol×K	332.70	Joback Method
cpg	110.28	J/mol×K	361.95	Joback Method

cpg	115.17	J/mol×K	391.19	Joback Method
cpg	119.94	J/mol×K	420.44	Joback Method
cpg	124.56	J/mol×K	449.68	Joback Method
cpg	129.05	J/mol×K	478.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.50 ± 0.50	K	97.30	NIST Webbook

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=C927800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
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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