

Ethynol

Inchi:	InChI=1S/C2H2O/c1-2-3/h1,3H
InchiKey:	QFXZANXYUCUTQH-UHFFFAOYSA-N
Formula:	C2H2O
SMILES:	C#CO
Mol. weight [g/mol]:	42.04
CAS:	32038-79-2

Physical Properties

Property code	Value	Unit	Source
gf	52.21	kJ/mol	Joback Method
hf	41.60	kJ/mol	NIST Webbook
hfus	8.00	kJ/mol	Joback Method
hvap	36.58	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	-0.050		Crippen Method
mcvol	36.310	ml/mol	McGowan Method
pc	7305.14	kPa	Joback Method
tb	327.46	K	Joback Method
tc	500.83	K	Joback Method
tf	220.09	K	Joback Method
vc	0.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	53.48	J/molxK	327.46	Joback Method
cpg	55.56	J/molxK	356.36	Joback Method
cpg	57.53	J/molxK	385.25	Joback Method
cpg	59.40	J/molxK	414.15	Joback Method
cpg	61.16	J/molxK	443.04	Joback Method
cpg	62.82	J/molxK	471.94	Joback Method
cpg	64.40	J/molxK	500.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32038792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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