2-Propynal

Other names:	Propyn-3-al
	Propiolaldehye
	Propargylaldehyde
	Propioaldehyde
	Propynal
	Propiolaldehyde
	2-Propyn-1-one
	Formylacetylene
	Acetylenecarboxaldehyde
Inchi:	InChI=1S/C3H2O/c1-2-3-4/h1,3H
InchiKey:	IJNJLGFTSIAHEA-UHFFFAOYSA-N
Formula:	C3H2O
SMILES:	C#CC=O
Mol. weight [g/mol]:	54.05
CAS:	624-67-9

Physical Properties

Property code	Value	Unit	Source
gf	97.93	kJ/mol	Joback Method
hf	101.07	kJ/mol	Joback Method
hfus	8.79	kJ/mol	Joback Method
hvap	28.85	kJ/mol	Joback Method
ie	10.62 ± 0.15	eV	NIST Webbook
ie	10.80	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
log10ws	-0.15		Crippen Method
logp	-0.182		Crippen Method
mcvol	46.100	ml/mol	McGowan Method
pc	6065.55	kPa	Joback Method
tb	333.20	K	NIST Webbook
tc	492.26	K	Joback Method
tf	212.54	K	Joback Method
vc	0.182	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	66.41	J/mol×K	306.82	Joback Method
cpg	69.48	J/mol×K	337.73	Joback Method
cpg	72.39	J/mol×K	368.63	Joback Method
cpg	75.14	J/mol×K	399.54	Joback Method
cpg	77.73	J/mol×K	430.44	Joback Method
cpg	80.18	J/mol×K	461.35	Joback Method
cpg	82.50	J/mol×K	492.26	Joback Method

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=C624679&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
ie:	Ionization energy
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