1-Propynol

Other names: CH3CCOH
Inchi: InChI=1S/C3H4O/c1-2-3-4/h4H,1H3
InchiKey: FWLKYEAOOIPJRL-UHFFFAOYSA-N
Formula: C3H4O
SMILES: CC#CO
Mol. weight [g/mol]: 56.06
CAS: 6175-54-8

Physical Properties

Property code	Value	Unit	Source
gf	40.36	kJ/mol	Joback Method
hf	14.82	kJ/mol	Joback Method
hfus	10.74	kJ/mol	Joback Method
hvap	41.10	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.340		Crippen Method
mcvol	50.400	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
tb	369.22	K	Joback Method
tc	555.66	K	Joback Method
tf	290.49	K	Joback Method
vc	0.184	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.97	J/mol×K	369.22	Joback Method
cpg	80.68	J/mol×K	400.29	Joback Method
cpg	84.26	J/mol×K	431.37	Joback Method
cpg	87.73	J/mol×K	462.44	Joback Method
cpg	91.08	J/mol×K	493.51	Joback Method
cpg	94.32	J/mol×K	524.59	Joback Method
cpg	97.45	J/mol×K	555.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6175548&Units=SI
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

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