5-Hexen-3-yn-2-ol, 2-methyl-

Other names: Dimethyl(vinylethynyl)carbinol
2-Methyl-5-hexen-3-yn-2-ol
Inchi: InChI=1S/C7H10O/c1-4-5-6-7(2,3)8/h4,8H,1H2,2-3H3
InchiKey: OYWGYGPXPDGOGH-UHFFFAOYSA-N
Formula: C7H10O
SMILES: C=CC#CC(C)(C)O
Mol. weight [g/mol]: 110.15
CAS: 690-94-8

Physical Properties

Property code	Value	Unit	Source
chl	-4169.20 ± 0.50	kJ/mol	NIST Webbook
gf	164.72	kJ/mol	Joback Method
hf	46.20 ± 0.80	kJ/mol	NIST Webbook
hfl	-14.60 ± 0.70	kJ/mol	NIST Webbook
hfus	12.40	kJ/mol	Joback Method
hvap	60.80	kJ/mol	NIST Webbook
hvap	60.80 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.78		Crippen Method
logp	0.947		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	454.19	K	Joback Method
tc	651.10	K	Joback Method
tf	336.23	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.15	J/mol×K	454.19	Joback Method
cpg	213.91	J/mol×K	487.01	Joback Method
cpg	223.09	J/mol×K	519.83	Joback Method
cpg	231.72	J/mol×K	552.64	Joback Method

cpg	239.83	J/mol×K	585.46	Joback Method
cpg	247.46	J/mol×K	618.28	Joback Method
cpg	254.62	J/mol×K	651.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C690948&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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