

3-Methyl-1-penten-4-yn-3-ol

Other names:	1-Penten-4-yn-3-ol, 3-methyl-3-Methyl-pent-4-en-1-yn-3-ol 3-Methyl pent-4-en-1-yn-3-ol 3-methylpent-1-en-4-yn-3-ol
Inchi:	InChI=1S/C6H8O/c1-4-6(3,7)5-2/h1,5,7H,2H2,3H3
InchiKey:	VBATUBQIYXCZPA-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	C#CC(C)(O)C=C
Mol. weight [g/mol]:	96.13
CAS:	3230-69-1

Physical Properties

Property code	Value	Unit	Source
chl	-3322.50 ± 1.70	kJ/mol	NIST Webbook
gf	176.57	kJ/mol	Joback Method
hf	89.18	kJ/mol	Joback Method
hfl	-181.90 ± 1.70	kJ/mol	NIST Webbook
hfus	9.66	kJ/mol	Joback Method
hvap	43.52	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.557		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	412.43	K	Joback Method
tc	599.34	K	Joback Method
tf	265.83	K	Joback Method
vc	0.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.03	J/mol×K	412.43	Joback Method
cpg	176.41	J/mol×K	443.58	Joback Method
cpg	184.24	J/mol×K	474.73	Joback Method

cpg	191.54	J/mol×K	505.88	Joback Method
cpg	198.35	J/mol×K	537.04	Joback Method
cpg	204.70	J/mol×K	568.19	Joback Method
cpg	210.63	J/mol×K	599.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3230691&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

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

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