1-Pentyn-3-ol, 3-methyl-

Other names:

(+/-)-3-Methylpent-1-yn-3-ol
2-Butanol, 2-ethynyl-
2-Ethinyl butanol-2
2-Ethynyl-2-butanol
3-Hydroxy-3-methyl-1-pentyne
3-Methyl-1-pentin-3-ol
3-Methyl-1-pentyn-3-ol
3-Methyl-1-pentyne-3-ol
3-Methyl-pentin-(1)-ol-(3)
3-Methylpent-1-yn-3-ol
3-Methylpentin-3-ol
3-Methylpentyn-3-ol
3-Metil-pentin-3-ol
Allotropal
Aniphor
Apridol
Atemorin
Atempol
BDH
Citodorm
Comesa
Dalgol
Dorison
Dormalest
Dormidin
Dormigen
Dormiphen
Dormison
Dormocit
Dormosan
Ethinylmethylethylcarbinol
Ethyl ethynyl methyl carbinol
Ethynylethylmethylcarbinol
Formison
Hesofen
Hexofen
Imnudorm
Insomnol
Macarol
Mecarol

Melpintol
Meparfynol
Mepentamato
Mepentil
Methylethylacetylenylcarbinol
Methylethylethynylcarbinol
Methylparafynol
Methylpentinol
Methylpentynol
Methylpentynolum
Metilparafinolo
Metilpentinolo
Miramel
N-Oblivon
Noxokratin
Oblevil
Oblivon
Oblivon C
Olfine P
Olosot
Olvadon
Pent-1-yne-3-ol, 3-methyl-
Pentadorm
Pentinol
Pentydorm
Pentydrom
Pentyrest
Perlopal
Placidal
Riposon
Sedapercut
Seral
Sintyal
Somnesin
Sonnormon
Trusono
Util
anti-Stress
«alpha»-Ethyl-«alpha»-methylpropargyl alcohol
Â«alphaÂ»-Ethyl-Â«alphaÂ»-methylpropargyl alcohol

Inchi: InChI=1S/C6H10O/c1-4-6(3,7)5-2/h1,7H,5H2,2-3H3

InchiKey: QXLPXWSKPNOQLE-UHFFFAOYSA-N

Formula: C6H10O

SMILES: C#CC(C)(O)CC
Mol. weight [g/mol]: 98.14
CAS: 77-75-8

Physical Properties

Property code	Value	Unit	Source
gf	88.73	kJ/mol	Joback Method
hf	-36.25	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
ie	10.03	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	0.781		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	715.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	690.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
ripol	1275.00		NIST Webbook
tb	393.70	K	NIST Webbook
tb	394.50 ± 0.50	K	NIST Webbook
tc	598.74	K	Joback Method
tf	267.59	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.97	J/mol×K	415.75	Joback Method
cpg	192.04	J/mol×K	446.25	Joback Method
cpg	200.58	J/mol×K	476.75	Joback Method
cpg	208.62	J/mol×K	507.24	Joback Method

cpg	216.18	J/mol×K	537.74	Joback Method
cpg	223.28	J/mol×K	568.24	Joback Method
cpg	229.97	J/mol×K	598.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64833e+01
Coeff. B	-4.07773e+03
Coeff. C	-5.08210e+01
Temperature range (K), min.	302.15
Temperature range (K), max.	416.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77758&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume