

1-Penten-3-ol, 3-methyl-

Other names:	(. +/-)-3-Methyl-1-penten-3-ol 3-Methyl-1-penten-3-ol 3-Methyl-penten-(1)-ol-(3) 3-methylpent-1-en-3-ol Ethylbutenol Methylethylvinylcarbinol
Inchi:	InChI=1S/C6H12O/c1-4-6(3,7)5-2/h4,7H,1,5H2,2-3H3
InchiKey:	HFYAEUXHCMTPOL-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=CC(C)(O)CC
Mol. weight [g/mol]:	100.16
CAS:	918-85-4

Physical Properties

Property code	Value	Unit	Source
gf	-46.50	kJ/mol	Joback Method
hf	-202.72	kJ/mol	Joback Method
hfus	6.69	kJ/mol	Joback Method
hvap	43.66	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	390.70	K	NIST Webbook
tc	596.78	K	Joback Method
tf	218.86	K	Joback Method
vc	0.360	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.52	J/molxK	422.31	Joback Method
cpg	204.52	J/molxK	451.39	Joback Method
cpg	213.99	J/molxK	480.47	Joback Method

cpg	222.96	J/molxK	509.55	Joback Method
cpg	231.44	J/molxK	538.63	Joback Method
cpg	239.47	J/molxK	567.71	Joback Method
cpg	247.07	J/molxK	596.78	Joback Method
dvisc	0.1218411	Paxs	218.86	Joback Method
dvisc	0.0223014	Paxs	252.77	Joback Method
dvisc	0.0060999	Paxs	286.68	Joback Method
dvisc	0.0021949	Paxs	320.59	Joback Method
dvisc	0.0009604	Paxs	354.49	Joback Method
dvisc	0.0004854	Paxs	388.40	Joback Method
dvisc	0.0002738	Paxs	422.31	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58994e+01
Coeff. B	-3.84626e+03
Coeff. C	-4.97510e+01
Temperature range (K), min.	295.70
Temperature range (K), max.	413.02

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C918854&Units=SI>

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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