4-Penten-2-ol, 4-methyl-

Other names:	4-Methyl-4-penten-2-ol
	4-methylpent-4-en-2-ol
Inchi:	InChI=1S/C6H12O/c1-5(2)4-6(3)7/h6-7H,1,4H2,2-3H3
InchiKey:	KPHPTSMXBAVNPX-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=C(C)CC(C)O
Mol. weight [g/mol]:	100.16
CAS:	2004-67-3

Physical Properties

Property code	Value	Unit	Source
gf	-60.33	kJ/mol	Joback Method
hf	-209.04	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	424.98	K	Joback Method
tc	595.89	K	Joback Method
tf	187.48	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.18	J/mol×K	424.98	Joback Method
cpg	201.51	J/mol×K	453.46	Joback Method
cpg	210.45	J/mol×K	481.95	Joback Method
cpg	219.01	J/mol×K	510.43	Joback Method
cpg	227.21	J/mol×K	538.92	Joback Method
cpg	235.05	J/mol×K	567.40	Joback Method
cpg	242.55	J/mol×K	595.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40577e+01
Coeff. B	-3.50754e+03
Coeff. C	-5.41990e+01
Temperature range (K), min.	295.70
Temperature range (K), max.	455.23

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2004673&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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/77-779-3/4-Penten-2-ol-4-methyl.pdf

Generated by Cheméo on 2024-10-12 07:01:47.109001197 +0000 UTC m=+3297369.745970454.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.