

4-Pentene-2-ol, 2-methyl

Other names:	CH2=CHCH2C(CH3)2OH 1-Pentene-4-ol, 4-methyl 4-Penten-2-ol, 2-methyl- 2-Methyl-4-penten-2-ol
Inchi:	InChI=1S/C6H12O/c1-4-5-6(2,3)7/h4,7H,1,5H2,2-3H3
InchiKey:	UYOPRNGQFQWYER-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=CCC(C)(C)O
Mol. weight [g/mol]:	100.16
CAS:	624-97-5

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	392.70	K	NIST Webbook
tc	596.78	K	Joback Method
tf	218.86	K	Joback Method
vc	0.360	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.52	J/mol×K	422.31	Joback Method
cpg	204.52	J/mol×K	451.39	Joback Method
cpg	213.99	J/mol×K	480.47	Joback Method
cpg	222.96	J/mol×K	509.55	Joback Method
cpg	231.44	J/mol×K	538.63	Joback Method

cpg	239.47	J/mol×K	567.71	Joback Method
cpg	247.07	J/mol×K	596.78	Joback Method
dvisc	0.1218411	Pa×s	218.86	Joback Method
dvisc	0.0223014	Pa×s	252.77	Joback Method
dvisc	0.0060999	Pa×s	286.68	Joback Method
dvisc	0.0021949	Pa×s	320.59	Joback Method
dvisc	0.0009604	Pa×s	354.49	Joback Method
dvisc	0.0004854	Pa×s	388.40	Joback Method
dvisc	0.0002738	Pa×s	422.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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