2-Propen-1-ol, 2-methyl-

Other names:	2-Methallyl alcohol
	2-Methyl-2-propen-1-ol
	2-Methyl-2-propene-1-ol
	2-Methyl-2-propenol
	2-Methylallyl alcohol
	2-Methylprop-2-en-1-ol
	3-Hydroxy-2-methylpropene
	CH2=C(CH3)CH2OH
	Isopropenyl carbinol
	Methacryl alcohol
	Methallyl alcohol
	NSC 30674
	UN 2614
	«beta»-Methallyl alcohol
	«beta»-Methylallyl alcohol
	Â«betaÂ»-Methallyl alcohol
	Â«betaÂ»-Methylallyl alcohol
Inchi:	InChI=1S/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3
InchiKey:	BYDRTKVGBRTTIT-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	C=C(C)CO
Mol. weight [g/mol]:	72.11
CAS:	513-42-8

Physical Properties

Property code	Value	Unit	Source
gf	-74.73	kJ/mol	Joback Method
hf	-162.48	kJ/mol	Joback Method
hfus	7.61	kJ/mol	Joback Method
hvap	51.90	kJ/mol	NIST Webbook
ie	9.24	eV	NIST Webbook
ie	9.28 ± 0.05	eV	NIST Webbook
log10ws	-0.61		Crippen Method
logp	0.555		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
rinpol	605.00		NIST Webbook

rinpol	633.00		NIST Webbook
rinpol	607.00		NIST Webbook
tb	387.70	K	NIST Webbook
tc	548.15	K	Joback Method
tf	179.94	K	Joback Method
vc	0.261	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.49	J/mol×K	379.66	Joback Method
cpg	127.00	J/mol×K	407.74	Joback Method
cpg	133.24	J/mol×K	435.82	Joback Method
cpg	139.22	J/mol×K	463.91	Joback Method
cpg	144.95	J/mol×K	491.99	Joback Method
cpg	150.45	J/mol×K	520.07	Joback Method
cpg	155.71	J/mol×K	548.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58560e+01
Coeff. B	-3.80711e+03
Coeff. C	-4.89170e+01
Temperature range (K), min.	293.46
Temperature range (K), max.	409.97

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C513428&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

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

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