3-Buten-1-ol, 2-methyl-

Other names: 2-Methyl-3-buten-1-ol
2-Methyl-3-butene-1-ol
2-Methyl-but-3-en-1-ol
Inchi: InChI=1S/C5H10O/c1-3-5(2)4-6/h3,5-6H,1,4H2,2H3
InchiKey: NVGOATMUHKIQQG-UHFFFAOYSA-N
Formula: C5H10O
SMILES: C=CC(C)CO
Mol. weight [g/mol]: 86.13
CAS: 4516-90-9

Physical Properties

Property code	Value	Unit	Source
gf	-60.20	kJ/mol	Joback Method
hf	-178.61	kJ/mol	Joback Method
hfus	7.99	kJ/mol	Joback Method
hvap	42.34	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	0.801		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	778.00		NIST Webbook
rinpol	778.00		NIST Webbook
tb	402.22	K	Joback Method
tc	570.76	K	Joback Method
tf	190.17	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.14	J/mol×K	402.22	Joback Method
cpg	163.12	J/mol×K	430.31	Joback Method
cpg	170.77	J/mol×K	458.40	Joback Method
cpg	178.10	J/mol×K	486.49	Joback Method

cpg	185.13	J/mol×K	514.58	Joback Method
cpg	191.86	J/mol×K	542.67	Joback Method
cpg	198.29	J/mol×K	570.76	Joback Method
dvisc	0.2702616	Pa×s	190.17	Joback Method
dvisc	0.0351986	Pa×s	225.51	Joback Method
dvisc	0.0079642	Pa×s	260.85	Joback Method
dvisc	0.0025691	Pa×s	296.19	Joback Method
dvisc	0.0010548	Pa×s	331.54	Joback Method
dvisc	0.0005141	Pa×s	366.88	Joback Method
dvisc	0.0002843	Pa×s	402.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.70	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58989e+01
Coeff. B	-3.87055e+03
Coeff. C	-5.05850e+01
Temperature range (K), min.	298.52
Temperature range (K), max.	416.16

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=C4516909&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume