3-Buten-2-ol

Other names:	1-Buten-3-ol
	1-Methyl-2-propenol
	3-Butene-2-ol
	3-Hydroxy-1-butene
	CH2=CHCH(OH)CH3
	Methyl vinylcarbinol
	Propenol, 1-methyl
	but-3-en-2-ol
Inchi:	InChI=1S/C4H8O/c1-3-4(2)5/h3-5H,1H2,2H3
InchiKey:	MKUWVMRNQOOSAT-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	C=CC(C)O
Mol. weight [g/mol]:	72.11
CAS:	598-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-68.62	kJ/mol	Joback Method
hf	-157.97	kJ/mol	Joback Method
hfus	5.40	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
ie	9.53	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.50 ± 0.05	eV	NIST Webbook
ie	10.05	eV	NIST Webbook
log10ws	-0.73		Crippen Method
logp	0.553		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	542.00		NIST Webbook
rinpol	543.00		NIST Webbook
tb	370.20	K	NIST Webbook
tb	370.15 ± 1.50	K	NIST Webbook
tc	548.41	K	Joback Method
tf	178.90	K	Joback Method
vc	0.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.44	J/mol×K	379.34	Joback Method
cpg	151.04	J/mol×K	520.24	Joback Method
cpg	145.44	J/mol×K	492.06	Joback Method
cpg	139.59	J/mol×K	463.88	Joback Method
cpg	133.47	J/mol×K	435.70	Joback Method
cpg	127.10	J/mol×K	407.52	Joback Method
cpg	156.40	J/mol×K	548.41	Joback Method
dvisc	0.0003283	Pa×s	379.34	Joback Method
dvisc	0.0006016	Pa×s	345.93	Joback Method
dvisc	0.0012550	Pa×s	312.53	Joback Method
dvisc	0.0031215	Pa×s	279.12	Joback Method
dvisc	0.0099469	Pa×s	245.71	Joback Method
dvisc	0.0456475	Pa×s	212.31	Joback Method
dvisc	0.3700665	Pa×s	178.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58984e+01
Coeff. B	-3.67896e+03
Coeff. C	-4.40520e+01
Temperature range (K), min.	279.72
Temperature range (K), max.	391.55

Sources

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=C598323&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

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
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