3-Buten-1-ol

Other names:	1-Buten-4-ol
	3-Buten-1-O1
	3-Butenyl alcohol
	Allylcarbinol
	BUTEN-(3)-O1-(L)
	But-3-en-1-ol
	CH2=CHCH2CH2OH
	Vinylethyl alcohol
Inchi:	InChI=1S/C4H8O/c1-2-3-4-5/h2,5H,1,3-4H2
InchiKey:	ZSPTYLOMNJNZNG-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	C=CCCO
Mol. weight [g/mol]:	72.11
CAS:	627-27-0

Physical Properties

Property code	Value	Unit	Source
gf	-66.18	kJ/mol	Joback Method
hf	-152.69	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	50.80	kJ/mol	NIST Webbook
ie	9.56 ± 0.05	eV	NIST Webbook
log10ws	-0.61		Crippen Method
logp	0.555		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
rinpol	620.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	597.00		NIST Webbook
rinpol	640.00		NIST Webbook

rinpol	620.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	596.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1137.00		NIST Webbook
ripol	1178.00		NIST Webbook
ripol	1149.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1171.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1187.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1209.00		NIST Webbook
tb	385.40 ± 2.00	K	NIST Webbook
tb	386.70	K	NIST Webbook
tb	387.00	K	NIST Webbook
tc	545.02	K	Joback Method
tf	193.90	K	Joback Method
vc	0.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.47	J/mol×K	379.78	Joback Method
cpg	126.89	J/mol×K	407.32	Joback Method
cpg	133.04	J/mol×K	434.86	Joback Method
cpg	138.95	J/mol×K	462.40	Joback Method
cpg	144.62	J/mol×K	489.94	Joback Method
cpg	150.05	J/mol×K	517.48	Joback Method
cpg	155.26	J/mol×K	545.02	Joback Method
dvisc	0.0235746	Pa×s	224.88	Joback Method
dvisc	0.1244334	Pa×s	193.90	Joback Method

dvisc	0.0066821	Pa×s	255.86	Joback Method
dvisc	0.0024869	Pa×s	286.84	Joback Method
dvisc	0.0011222	Pa×s	317.82	Joback Method
dvisc	0.0005833	Pa×s	348.80	Joback Method
dvisc	0.0003373	Pa×s	379.78	Joback Method
hvapt	50.90 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	48.80 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	46.70 ± 0.10	kJ/mol	343.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58992e+01
Coeff. B	-3.81362e+03
Coeff. C	-4.86390e+01
Temperature range (K), min.	292.92
Temperature range (K), max.	408.83

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=C627270&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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume