

2-Buten-1-ol

Other names:	1-Hydroxy-2-butene 2-Butene-1-ol 2-Butenol 2-Butenyl alcohol 2-buten-1-ol (crotyl alcohol) 3-Methylallyl alcohol CH3CH=CHCH2OH Crotonyl alcohol Crotyl alcohol Krotylalkohol NSC 17480 but-2-en-1-ol
Inchi:	InChI=1S/C4H8O/c1-2-3-4-5/h2-3,5H,4H2,1H3
InchiKey:	WCASXYBKJHWFMY-UHFFFAOYSA-N
Formula:	C4H8O
SMILES:	CC=CCO
Mol. weight [g/mol]:	72.11
CAS:	6117-91-5

Physical Properties

Property code	Value	Unit	Source
gf	-73.80	kJ/mol	Joback Method
hf	-160.90	kJ/mol	Joback Method
hfus	10.41	kJ/mol	Joback Method
hvap	41.14	kJ/mol	Joback Method
ie	9.13	eV	NIST Webbook
log10ws	-0.61		Crippen Method
logp	0.555		Crippen Method
mcvol	68.790	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
rinpol	628.00		NIST Webbook
rinpol	625.00		NIST Webbook
rinpol	657.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	650.00		NIST Webbook
rinpol	664.00		NIST Webbook

rinpol	653.00		NIST Webbook
ripol	1193.00		NIST Webbook
ripol	1193.00		NIST Webbook
tb	394.70	K	NIST Webbook
tc	557.54	K	Joback Method
tf	190.58	K	Joback Method
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.16	J/mol×K	387.26	Joback Method
cpg	125.85	J/mol×K	415.64	Joback Method
cpg	132.23	J/mol×K	444.02	Joback Method
cpg	138.32	J/mol×K	472.40	Joback Method
cpg	144.13	J/mol×K	500.78	Joback Method
cpg	149.66	J/mol×K	529.16	Joback Method
cpg	154.94	J/mol×K	557.54	Joback Method
dvisc	0.1526839	Pa×s	190.58	Joback Method
dvisc	0.0243706	Pa×s	223.36	Joback Method
dvisc	0.0062218	Pa×s	256.14	Joback Method
dvisc	0.0021653	Pa×s	288.92	Joback Method
dvisc	0.0009344	Pa×s	321.70	Joback Method
dvisc	0.0004710	Pa×s	354.48	Joback Method
dvisc	0.0002666	Pa×s	387.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58995e+01
Coeff. B	-3.87890e+03
Coeff. C	-5.08630e+01
Temperature range (K), min.	299.32
Temperature range (K), max.	417.21

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=C6117915&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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