

2-Butene-1,4-diol, (Z)-

Other names:	(Z)-2-BUTENE-1,4-DIOL CIS-2-BUTENE-1,4-DIOL CIS-BUTENEDIOL cis-1,4-Dihydroxy-2-butene
Inchi:	InChI=1S/C4H8O2/c5-3-1-2-4-6/h1-2,5-6H,3-4H2/b2-1-
InchiKey:	ORTVZLZNOYNASJ-UPHRSURJSA-N
Formula:	C4H8O2
SMILES:	OCC=CCO
Mol. weight [g/mol]:	88.11
CAS:	6117-80-2

Physical Properties

Property code	Value	Unit	Source
gf	-210.62	kJ/mol	Joback Method
hf	-313.13	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	57.81	kJ/mol	Joback Method
log10ws	0.12		Crippen Method
logp	-0.473		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
tb	508.20	K	NIST Webbook
tc	644.82	K	Joback Method
tf	284.20 ± 0.50	K	NIST Webbook
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.90	J/molxK	644.82	Joback Method
cpg	182.26	J/molxK	617.25	Joback Method
cpg	177.40	J/molxK	589.69	Joback Method
cpg	172.30	J/molxK	562.13	Joback Method
cpg	166.95	J/molxK	534.57	Joback Method

cpg	161.35	J/molxK	507.00	Joback Method
cpg	155.46	J/molxK	479.44	Joback Method
dvisc	0.2463890	Paxs	251.40	Joback Method
dvisc	0.0001049	Paxs	479.44	Joback Method
dvisc	0.0002191	Paxs	441.43	Joback Method
dvisc	0.0005259	Paxs	403.43	Joback Method
dvisc	0.0015145	Paxs	365.42	Joback Method
dvisc	0.0055752	Paxs	327.41	Joback Method
dvisc	0.0289003	Paxs	289.41	Joback Method
hvapt	74.70	kJ/mol	440.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.06264e+01
Coeff. B	-8.33944e+03
Coeff. C	1.27540e+01
Temperature range (K), min.	397.27
Temperature range (K), max.	531.78

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	2.11722e+02
Coeff. B	-1.71176e+04
Coeff. C	-2.86125e+01
Coeff. D	1.87469e-05
Temperature range (K), min.	284.15
Temperature range (K), max.	677.88

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.therich.org/research/kdb/hcprop/showprop.php?cmpid=914
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6117802&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.therich.org/research/kdb/hcprop/showprop.php?cmpid=914
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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