2-Butene-1,4-diol

Other names:	1,4-Butenediol
	1,4-Dihydroxy-2-butene
	2-Buten-1,4-diol
	2-Butene, 1,4-dihydroxy-
	2-Butene-1,4-diol,c&t
	Butenediol
	but-2-ene-1,4-diol
Inchi:	InChI=1S/C4H8O2/c5-3-1-2-4-6/h1-2,5-6H,3-4H2
InchiKey:	ORTVZLZNOYNASJ-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	OCC=CCO
Mol. weight [g/mol]:	88.11
CAS:	110-64-5

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
rinpol	911.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	911.00		NIST Webbook
ripol	1983.00		NIST Webbook
tb	479.44	K	Joback Method
tc	644.82	K	Joback Method
tf	251.40	K	Joback Method
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.46	J/mol×K	479.44	Joback Method
cpg	161.35	J/mol×K	507.00	Joback Method
cpg	166.95	J/mol×K	534.57	Joback Method
cpg	172.30	J/mol×K	562.13	Joback Method
cpg	177.40	J/mol×K	589.69	Joback Method
cpg	182.26	J/mol×K	617.25	Joback Method
cpg	186.90	J/mol×K	644.82	Joback Method
dvisc	0.2463890	Pa×s	251.40	Joback Method
dvisc	0.0289003	Pa×s	289.41	Joback Method
dvisc	0.0055752	Pa×s	327.41	Joback Method
dvisc	0.0015145	Pa×s	365.42	Joback Method
dvisc	0.0005259	Pa×s	403.43	Joback Method
dvisc	0.0002191	Pa×s	441.43	Joback Method
dvisc	0.0001049	Pa×s	479.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.17161e+01
Coeff. B	-2.92436e+03
Coeff. C	-5.46040e+01
Temperature range (K), min.	310.49
Temperature range (K), max.	511.20

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110645&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	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