1,2,4-Butanetriol

Other names:	1,2,4-Butantriol
	1,2,4-trihydroxybutane
	1,3,4-butanetriol
	2-Deoxyerythritol
	Butane-1,2,4-triol
	HOCH2CH(OH)CH2CH2OH
	Triol 124
Inchi:	InChI=1S/C4H10O3/c5-2-1-4(7)3-6/h4-7H,1-3H2
InchiKey:	ARXKVVRQIIOZGF-UHFFFAOYSA-N
Formula:	C4H10O3
SMILES:	OCCC(O)CO
Mol. weight [g/mol]:	106.12
CAS:	3068-00-6

Physical Properties

Property code	Value	Unit	Source
affp	905.90	kJ/mol	NIST Webbook
basg	841.00	kJ/mol	NIST Webbook
gf	-430.10	kJ/mol	Joback Method
hf	-587.86	kJ/mol	Joback Method
hfus	14.86	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	0.60		Crippen Method
logp	-1.278		Crippen Method
mcvol	84.830	ml/mol	McGowan Method
pc	5756.64	kPa	Joback Method
tb	567.02	K	Joback Method
tc	725.28	K	Joback Method
tf	302.30	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	211.49	J/mol×K	567.02	Joback Method
cpg	217.38	J/mol×K	593.40	Joback Method
cpg	223.03	J/mol×K	619.77	Joback Method
cpg	228.44	J/mol×K	646.15	Joback Method
cpg	233.64	J/mol×K	672.52	Joback Method
cpg	238.61	J/mol×K	698.90	Joback Method
cpg	243.37	J/mol×K	725.28	Joback Method
dvisc	0.1910150	Pa×s	302.30	Joback Method
dvisc	0.0160153	Pa×s	346.42	Joback Method
dvisc	0.0023509	Pa×s	390.54	Joback Method
dvisc	0.0005095	Pa×s	434.66	Joback Method
dvisc	0.0001463	Pa×s	478.78	Joback Method
dvisc	0.0000519	Pa×s	522.90	Joback Method
dvisc	0.0000216	Pa×s	567.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.70	K	2.40	NIST Webbook
tbrp	440.50 ± 0.50	K	1.50	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Isopiestic determination of osmotic and activity coefficients of aqueous solutions of aliphatic polyols at 298.15K: https://www.doi.org/10.1016/j.fluid.2005.12.016

Enthalpies of dilution of aqueous solutions of n-butanol, butanediols, 1,2,4-butanetriol, and 1,2,3,4-butanetetrol at 298.15K: https://www.doi.org/10.1016/j.tca.2005.06.014

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=C3068006&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity

basg: Gas basicity

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume