1,3-butanediol, DL-

Other names:	«beta»-Butylene glycol
	Methyltrimethylene glycol
	1-Methyl-1,3-propanediol
	1,3-Butylene glycol
	1,3-Dihydroxybutane
	Butane-1,3-diol
	BD
	1,3-Butandiol
	1,3-Butylenglykol
	1,3-Butanodiol
	Butanediol,1,3-
	(RS)-1,3-Butanediol
	Butylene glycol
	NSC 402145
	1,3-butanediol, DL-
Inchi:	InChI=1S/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3
InchiKey:	PUPZLCDOIYMWBV-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CC(O)CCO
Mol. weight [g/mol]:	90.12

Physical Properties

Property code	Value	Unit	Source
af	0.6814		Cheméo Relay (1.0)
gf	-293.28	kJ/mol	Joback Method
hf	-456.85	kJ/mol	Cheméo Relay (1.0)
hfus	10.77	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Cheméo Relay (1.0)
ie	10.06	eV	Cheméo Relay (1.0)
log10ws	0.76		Cheméo Relay (1.0)
logp	-0.250		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	4020.00 ± 250.00	kPa	NIST Webbook
rhoc	294.79 ± 11.72	kg/m3	NIST Webbook
tb	475.73	K	Cheméo Relay (1.0)
tc	676.00 ± 2.00	K	NIST Webbook
tf	244.33	K	Cheméo Relay (1.0)

vc	0.293	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.31	J/mol×K	474.84	Joback Method
cpg	179.93	J/mol×K	501.78	Joback Method
cpg	186.29	J/mol×K	528.72	Joback Method
cpg	192.41	J/mol×K	555.66	Joback Method
cpg	198.29	J/mol×K	582.59	Joback Method
cpg	203.94	J/mol×K	609.53	Joback Method
cpg	209.35	J/mol×K	636.47	Joback Method
dvisc	0.6060212	Pa×s	241.48	Joback Method
dvisc	0.0554139	Pa×s	280.37	Joback Method
dvisc	0.0090753	Pa×s	319.27	Joback Method
dvisc	0.0022017	Pa×s	358.16	Joback Method
dvisc	0.0007050	Pa×s	397.05	Joback Method
dvisc	0.0002766	Pa×s	435.95	Joback Method
dvisc	0.0001265	Pa×s	474.84	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18826954&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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

Legend

af: Acentric Factor

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
rhoc:	Critical density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume