1,3-Butanediol

Other names:	(RS)-1,3-Butanediol
	1,3-Butandiol
	1,3-Butanodiol
	1,3-Butylene glycol
	1,3-Butylenglykol
	1,3-Dihydroxybutane
	1-Methyl-1,3-propanediol
	BD
	Butane-1,3-diol
	Butanediol,1,3-
	Butylene glycol
	Methyltrimethylene glycol
	NSC 402145
	«beta»-Butylene glycol
	Â«betaÂ»-Butylene glycol
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
CAS:	107-88-0

Physical Properties

Property code	Value	Unit	Source
chl	-2502.20 ± 2.10	kJ/mol	NIST Webbook
chl	-2488.00	kJ/mol	NIST Webbook
ea	0.01 ± 0.00	eV	NIST Webbook
gf	-293.28	kJ/mol	Joback Method
hf	-433.00 ± 3.00	kJ/mol	NIST Webbook
hf	-447.10	kJ/mol	NIST Webbook
hfl	-515.10	kJ/mol	NIST Webbook
hfl	-501.00 ± 2.00	kJ/mol	NIST Webbook
hfus	10.77	kJ/mol	Joback Method
hvap	72.80 ± 0.60	kJ/mol	NIST Webbook
hvap	72.60 ± 0.30	kJ/mol	NIST Webbook
hvap	68.00	kJ/mol	NIST Webbook
hvap	74.50 ± 1.00	kJ/mol	NIST Webbook

log10ws	-0.14		Crippen Method
logp	-0.250		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	788.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1556.00		NIST Webbook
tb	480.65 ± 0.70	K	NIST Webbook
tb	481.15 ± 1.00	K	NIST Webbook
tb	478.65 ± 3.00	K	NIST Webbook
tb	481.43 ± 0.05	K	NIST Webbook
tb	480.15 ± 1.00	K	NIST Webbook
tb	480.65 ± 1.00	K	NIST Webbook
tb	480.15 ± 1.00	K	NIST Webbook
tb	476.70	K	NIST Webbook
tc	636.47	K	Joback Method

tf	241.48	K	Joback Method
vc	0.291	m3/kmol	Joback Method

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
cpl	227.20	J/mol×K	303.00	NIST Webbook
dvisc	0.0001265	Pa×s	474.84	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	0.6060212	Pa×s	241.48	Joback Method
dvisc	0.0002766	Pa×s	435.95	Joback Method
dvisc	0.0007050	Pa×s	397.05	Joback Method
hvapt	72.30 ± 0.80	kJ/mol	441.50	NIST Webbook
hvapt	68.30 ± 0.70	kJ/mol	441.50	NIST Webbook
hvapt	64.10 ± 0.60	kJ/mol	441.50	NIST Webbook
hvapt	59.50 ± 0.50	kJ/mol	441.50	NIST Webbook
hvapt	54.40 ± 0.60	kJ/mol	441.50	NIST Webbook
hvapt	67.60	kJ/mol	422.50	NIST Webbook
hvapt	68.00 ± 2.00	kJ/mol	373.00	NIST Webbook
hvapt	59.70	kJ/mol	398.00	NIST Webbook
hvapt	58.10	kJ/mol	451.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.93946e+02
Coeff. B	-1.61131e+04

Coeff. C	-2.58392e+01
Coeff. D	1.62357e-05
Temperature range (K), min.	196.15
Temperature range (K), max.	643.00

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107880&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=917
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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