1,2-Butanediol

Other names:	1,2-Butylene glycol
	«alpha»-Butylene glycol
	Ethylethylene glycol
	1,2-(Dihydroxy)butane
	Butane-1,2-diol
	DL-1,2-Butanediol
	1,2-Butandiol
	NSC 24242
Inchi:	InChI=1S/C4H10O2/c1-2-4(6)3-5/h4-6H,2-3H2,1H3
InchiKey:	BMRWNKZVCUKKSR-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CCC(O)CO
Mol. weight [g/mol]:	90.12
CAS:	584-03-2

Physical Properties

Property code	Value	Unit	Source
chl	-2479.00	kJ/mol	NIST Webbook
gf	-293.28	kJ/mol	Joback Method
hf	-435.63	kJ/mol	Joback Method
hfl	-523.80	kJ/mol	NIST Webbook
hfus	10.77	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.250		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
rinpol	809.00		NIST Webbook
rinpol	809.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	812.80		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1563.00		NIST Webbook
tb	469.65 ± 2.00	K	NIST Webbook
tb	463.65 ± 1.00	K	NIST Webbook
tb	463.65 ± 1.00	K	NIST Webbook
tb	456.65 ± 6.00	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
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

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=C584032&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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