

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 1,2-Butanediol, (.+/-.)-
Inchi:	InChI=1S/C4H10O2/c1-2-4(6)3-5/h4-6H,2-3H2,1H3
InchiKey:	BMRWKNKZVCUKKSR-UHFFFAOYSA-N
Formula:	C4H10O2
SMILES:	CCC(O)CO
Mol. weight [g/mol]:	90.12
CAS:	26171-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-293.28	kJ/mol	Joback Method
hf	-435.63	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	73.30 ± 0.40	kJ/mol	NIST Webbook
hvap	70.40 ± 0.30	kJ/mol	NIST Webbook
hvap	71.60 ± 0.80	kJ/mol	NIST Webbook
log10ws	-0.14		Crippen Method
logp	-0.250		Crippen Method
mcvol	78.960	ml/mol	McGowan Method
pc	5210.00 ± 250.00	kPa	NIST Webbook
rhoc	297.40 ± 11.72	kg/m3	NIST Webbook
tb	474.84	K	Joback Method
tc	680.00 ± 2.00	K	NIST Webbook
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	0.0001265	Pa×s	474.84	Joback Method
dvisc	0.0554139	Pa×s	280.37	Joback Method
dvisc	0.6060212	Pa×s	241.48	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	0.0090753	Pa×s	319.27	Joback Method
hvapt	51.50 ± 0.40	kJ/mol	439.00	NIST Webbook
hvapt	48.90 ± 0.40	kJ/mol	439.00	NIST Webbook
hvapt	46.30 ± 0.40	kJ/mol	439.00	NIST Webbook
hvapt	43.60 ± 0.40	kJ/mol	439.00	NIST Webbook
hvapt	40.70 ± 0.50	kJ/mol	439.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	464.70	K	99.60	NIST Webbook

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=C26171835&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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