

1,3-Butanediol, (R)-

Other names:	(R)-(-)-butane-1,3-diol
Inchi:	InChI=1S/C4H10O2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3/t4-/m0/s1
InchiKey:	PUPZLCDOIYMWBV-BYPYZUCNSA-N
Formula:	C4H10O2
SMILES:	CC(O)CCO
Mol. weight [g/mol]:	90.12
CAS:	6290-03-5

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	72.30 ± 0.70	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
tb	474.84	K	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.70	K	3.10	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=C6290035&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
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

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