

1,4-Butanediol, 2-methyl-

Other names:	2-methylbutane-1,4-diol
Inchi:	InChI=1S/C5H12O2/c1-5(4-7)2-3-6/h5-7H,2-4H2,1H3
InchiKey:	MWCBGWLCXSUTHK-UHFFFAOYSA-N
Formula:	C5H12O2
SMILES:	CC(CO)CCO
Mol. weight [g/mol]:	104.15
CAS:	2938-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-284.86	kJ/mol	Joback Method
hf	-456.27	kJ/mol	Joback Method
hfus	13.36	kJ/mol	Joback Method
hvap	59.69	kJ/mol	Joback Method
log10ws	-0.20		Crippen Method
logp	-0.003		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	398.15 ± 2.00	K	NIST Webbook
tb	466.15 ± 3.00	K	NIST Webbook
tc	658.58	K	Joback Method
tf	252.75	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.31	J/molxK	497.72	Joback Method
cpg	220.99	J/molxK	524.53	Joback Method
cpg	228.37	J/molxK	551.34	Joback Method
cpg	235.47	J/molxK	578.15	Joback Method
cpg	242.28	J/molxK	604.96	Joback Method
cpg	248.82	J/molxK	631.77	Joback Method
cpg	255.10	J/molxK	658.58	Joback Method

dvisc	0.3861453	Paxs	252.75	Joback Method
dvisc	0.0370842	Paxs	293.58	Joback Method
dvisc	0.0063110	Paxs	334.41	Joback Method
dvisc	0.0015790	Paxs	375.24	Joback Method
dvisc	0.0005185	Paxs	416.06	Joback Method
dvisc	0.0002078	Paxs	456.89	Joback Method
dvisc	0.0000967	Paxs	497.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2938989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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