

1-Butanol, 2-methyl-

Other names:	2-Methyl butanol-1
	2-Methyl-1-butanol
	2-Methyl-butan-1-ol
	2-Methyl-n-butanol
	2-Methylbutanol
	2-Methylbutyl alcohol
	2-methyl-1-butanol (active amyl alcohol)
	3-Methyl iso-butanol
	Active amyl alcohol
	Active primary amyl alcohol
	Butanol, 2-methyl-
	CH3CH2CH(CH3)CH2OH
	Methyl-2-butan-1-ol
	NSC 8431
	Primary active amyl alcohol
	dl-2-Methyl-1-butanol
	dl-sec-Butyl carbinol
Inchi:	InChI=1S/C5H12O/c1-3-5(2)4-6/h5-6H,3-4H2,1-2H3
InchiKey:	QPRQEDXDYOZYLA-UHFFFAOYSA-N
Formula:	C5H12O
SMILES:	CCC(C)CO
Mol. weight [g/mol]:	88.15
CAS:	137-32-6

Physical Properties

Property code	Value	Unit	Source
chl	-3325.90 ± 0.54	kJ/mol	NIST Webbook
gf	-148.04	kJ/mol	Joback Method
hf	-302.00 ± 1.50	kJ/mol	NIST Webbook
hfl	-356.60 ± 0.63	kJ/mol	NIST Webbook
hfus	9.27	kJ/mol	Joback Method
hvap	54.10	kJ/mol	NIST Webbook
hvap	54.60 ± 1.30	kJ/mol	NIST Webbook
hvap	54.60	kJ/mol	NIST Webbook
ie	9.86	eV	NIST Webbook

log10ws	-0.47		Estimated Solubility Method
logp	1.025		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3940.00 ± 20.00	kPa	NIST Webbook
pc	3940.00 ± 40.00	kPa	NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	738.00		NIST Webbook
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ripol	1210.00		NIST Webbook
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ripol	1210.00		NIST Webbook
tb	402.15 ± 1.00	K	NIST Webbook
tb	401.15 ± 2.00	K	NIST Webbook
tb	403.15 ± 2.00	K	NIST Webbook
tb	403.20	K	NIST Webbook
tb	402.05	K	NIST Webbook
tb	401.75 ± 0.50	K	NIST Webbook
tb	401.65 ± 2.00	K	NIST Webbook
tb	402.05 ± 0.30	K	NIST Webbook
tb	401.65 ± 1.00	K	NIST Webbook
tb	401.40 ± 0.50	K	NIST Webbook
tb	401.95 ± 0.50	K	NIST Webbook
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tb	400.65 ± 2.00	K	NIST Webbook
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tb	399.15 ± 2.00	K	NIST Webbook
tb	402.15 ± 1.00	K	NIST Webbook
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tb	402.15 ± 2.00	K	NIST Webbook
tb	402.55 ± 0.50	K	NIST Webbook
tb	400.65 ± 2.00	K	NIST Webbook
tb	401.15 ± 2.00	K	NIST Webbook
tb	401.15 ± 2.00	K	NIST Webbook
tb	401.65 ± 2.00	K	NIST Webbook
tb	401.15 ± 2.00	K	NIST Webbook
tc	575.40 ± 0.50	K	NIST Webbook
tc	575.40 ± 0.70	K	NIST Webbook
tf	191.93	K	Joback Method
vc	0.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.82	J/mol×K	405.54	Joback Method
cpg	178.43	J/mol×K	433.08	Joback Method
cpg	186.73	J/mol×K	460.61	Joback Method
cpg	194.72	J/mol×K	488.15	Joback Method
cpg	202.42	J/mol×K	515.68	Joback Method
cpg	209.82	J/mol×K	543.22	Joback Method
cpg	216.94	J/mol×K	570.76	Joback Method
dvisc	0.0002833	Pa×s	405.54	Joback Method
dvisc	0.0379452	Pa×s	227.53	Joback Method
dvisc	0.0083860	Pa×s	263.13	Joback Method
dvisc	0.3005917	Pa×s	191.93	Joback Method
dvisc	0.0010745	Pa×s	334.34	Joback Method
dvisc	0.0005174	Pa×s	369.94	Joback Method
dvisc	0.0026559	Pa×s	298.74	Joback Method
hvapt	43.40	kJ/mol	356.00	NIST Webbook
hvapt	51.20	kJ/mol	367.50	NIST Webbook
hvapt	49.80	kJ/mol	370.00	NIST Webbook
hvapt	53.90	kJ/mol	360.00	NIST Webbook
hvapt	58.50	kJ/mol	284.00	NIST Webbook
hvapt	56.70	kJ/mol	345.50	NIST Webbook
hvapt	56.10	kJ/mol	355.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C137326&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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