2-Butanol, 2,3-dimethyl-

Other names:	(CH3)2CHC(OH)(CH3)2
	2,3-Dimethyl-2-butanol
	2,3-dimethylbutan-2-ol
	Isopropyldimethylcarbinol
	Thexyl alcohol
Inchi:	InChI=1S/C6H14O/c1-5(2)6(3,4)7/h5,7H,1-4H3
InchiKey:	IKECULIHBUCAKR-UHFFFAOYSA-N
Formula:	C6H14O
SMILES:	CC(C)C(C)(C)O
Mol. weight [g/mol]:	102.17
CAS:	594-60-5

Physical Properties

Property code	Value	Unit	Source
gf	-136.78	kJ/mol	Joback Method
hf	-357.00 ± 0.59	kJ/mol	NIST Webbook
hfl	-411.00 ± 1.50	kJ/mol	NIST Webbook
hfus	4.45	kJ/mol	Joback Method
hvap	54.00	kJ/mol	NIST Webbook
hvap	54.00 ± 0.80	kJ/mol	NIST Webbook
hvap	54.02 ± 0.84	kJ/mol	NIST Webbook
log10ws	-0.41		Aqueous Solubility Prediction Method
logp	1.413		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	725.00		NIST Webbook
rinpol	716.30		NIST Webbook
rinpol	715.20		NIST Webbook
rinpol	714.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1082.00		NIST Webbook
tb	425.19	K	Joback Method
tc	600.02	K	Joback Method
tf	262.60 ± 0.30	K	NIST Webbook

tf	262.75 ± 0.20	K	NIST Webbook
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.06	J/mol×K	425.19	Joback Method
cpg	220.98	J/mol×K	454.33	Joback Method
cpg	231.37	J/mol×K	483.47	Joback Method
cpg	241.24	J/mol×K	512.60	Joback Method
cpg	250.62	J/mol×K	541.74	Joback Method
cpg	259.53	J/mol×K	570.88	Joback Method
cpg	267.98	J/mol×K	600.02	Joback Method
dvisc	0.0427885	Pa×s	242.22	Joback Method
dvisc	0.3533787	Pa×s	205.62	Joback Method
dvisc	0.0090180	Pa×s	278.81	Joback Method
dvisc	0.0027278	Pa×s	315.40	Joback Method
dvisc	0.0010580	Pa×s	352.00	Joback Method
dvisc	0.0004905	Pa×s	388.60	Joback Method
dvisc	0.0002596	Pa×s	425.19	Joback Method
hvapt	48.80	kJ/mol	349.50	NIST Webbook
hvapt	49.10	kJ/mol	345.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	337.70	K	11.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41799e+01
Coeff. B	-2.82134e+03

Coeff. C	-9.69280e+01
Temperature range (K), min.	300.02
Temperature range (K), max.	415.06

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594605&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume