1-Butanol, 2-methyl-, (S)-

Other names: (S)-(-)-2-Methyl-1-butanol
(S)-2-methylbutan-1-ol
l-2-Methyl-1-butanol
Inchi: InChI=1S/C5H12O/c1-3-5(2)4-6/h5-6H,3-4H2,1-2H3/t5-/m1/s1
InchiKey: QPRQEDXDYOZYLA-RXMQYKEDSA-N
Formula: C5H12O
SMILES: CCC(C)CO
Mol. weight [g/mol]: 88.15
CAS: 1565-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-148.04	kJ/mol	Joback Method
hf	-304.04	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	1.025		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	405.54	K	Joback Method
tc	570.76	K	Joback Method
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	0.3005917	Pa×s	191.93	Joback Method
dvisc	0.0379452	Pa×s	227.53	Joback Method
dvisc	0.0083860	Pa×s	263.13	Joback Method
dvisc	0.0026559	Pa×s	298.74	Joback Method
dvisc	0.0010745	Pa×s	334.34	Joback Method
dvisc	0.0005174	Pa×s	369.94	Joback Method
dvisc	0.0002833	Pa×s	405.54	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64817e+01
Coeff. B	-4.13271e+03
Coeff. C	-5.26420e+01
Temperature range (K), min.	307.84
Temperature range (K), max.	422.62

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C1565806&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume