2-Butanol, 3-methyl-, (S)-

Other names: (S)-(+)-3-Methyl-2-butanol
Inchi: InChI=1S/C5H12O/c1-4(2)5(3)6/h4-6H,1-3H3/t5-/m1/s1
InchiKey: MXLMTQWGSQIYOW-RXMQYKEDSA-N
Formula: C5H12O
SMILES: CC(C)C(C)O
Mol. weight [g/mol]: 88.15
CAS: 1517-66-4

Physical Properties

Property code	Value	Unit	Source
gf	-150.48	kJ/mol	Joback Method
hf	-309.32	kJ/mol	Joback Method
hfus	5.75	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.023		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	3955.54	kPa	Joback Method
tb	405.10	K	Joback Method
tc	574.03	K	Joback Method
tf	176.93	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.84	J/mol×K	405.10	Joback Method
cpg	211.03	J/mol×K	545.87	Joback Method
cpg	203.43	J/mol×K	517.72	Joback Method
cpg	195.52	J/mol×K	489.56	Joback Method
cpg	187.29	J/mol×K	461.41	Joback Method
cpg	178.73	J/mol×K	433.25	Joback Method
cpg	218.33	J/mol×K	574.03	Joback Method
dvisc	0.0002739	Pa×s	405.10	Joback Method

dvisc	0.0005293	Pa×s	367.07	Joback Method
dvisc	0.0011912	Pa×s	329.04	Joback Method
dvisc	0.0033141	Pa×s	291.01	Joback Method
dvisc	0.0125411	Pa×s	252.99	Joback Method
dvisc	0.0759974	Pa×s	214.96	Joback Method
dvisc	0.9991270	Pa×s	176.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	97.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1517664&Units=SI
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

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