2-Butanol, 3-methoxy-

Other names: 3-Methoxybutan-2-ol
3-methoxy-2-butanol
Inchi: InChI=1S/C5H12O2/c1-4(6)5(2)7-3/h4-6H,1-3H3
InchiKey: HJHFJCUIVDTESF-UHFFFAOYSA-N
Formula: C5H12O2
SMILES: COC(C)C(C)O
Mol. weight [g/mol]: 104.15
CAS: 53778-72-6

Physical Properties

Property code	Value	Unit	Source
gf	-255.48	kJ/mol	Joback Method
hf	-441.54	kJ/mol	Joback Method
hfus	6.94	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	0.402		Crippen Method
mcvol	93.050	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
ripol	1903.00		NIST Webbook
ripol	1910.00		NIST Webbook
tb	427.52	K	Joback Method
tc	596.57	K	Joback Method
tf	199.16	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.43	J/mol×K	427.52	Joback Method
cpg	232.27	J/mol×K	568.39	Joback Method
cpg	224.64	J/mol×K	540.22	Joback Method
cpg	216.75	J/mol×K	512.04	Joback Method
cpg	208.58	J/mol×K	483.87	Joback Method

cpg	200.14	J/mol×K	455.69	Joback Method
cpg	239.62	J/mol×K	596.57	Joback Method
dvisc	0.0002097	Pa×s	427.52	Joback Method
dvisc	0.0003885	Pa×s	389.46	Joback Method
dvisc	0.0008229	Pa×s	351.40	Joback Method
dvisc	0.0020914	Pa×s	313.34	Joback Method
dvisc	0.0068795	Pa×s	275.28	Joback Method
dvisc	0.0331601	Pa×s	237.22	Joback Method
dvisc	0.2915719	Pa×s	199.16	Joback Method

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=C53778726&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume