3-Methoxy-3-methylbutanol

Other names: 1-Butanol, 3-methoxy-3-methyl-
3-Methyl-3-methoxy-1-butanol
3-methoxy-3-methylbutan-1-ol
Inchi: InChI=1S/C6H14O2/c1-6(2,8-3)4-5-7/h7H,4-5H2,1-3H3
InchiKey: MFKRHJVUCZRDTF-UHFFFAOYSA-N
Formula: C6H14O2
SMILES: COC(C)(C)CCO
Mol. weight [g/mol]: 118.17
CAS: 56539-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-239.34	kJ/mol	Joback Method
hf	-460.37	kJ/mol	Joback Method
hfus	9.16	kJ/mol	Joback Method
hvap	46.74	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.794		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
ripol	1434.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	448.05	K	Joback Method
tc	618.94	K	Joback Method
tf	242.85	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.93	J/mol×K	448.05	Joback Method
cpg	280.27	J/mol×K	590.46	Joback Method
cpg	271.62	J/mol×K	561.97	Joback Method
cpg	262.58	J/mol×K	533.49	Joback Method

cpg	253.13	J/mol×K	505.01	Joback Method
cpg	243.25	J/mol×K	476.53	Joback Method
cpg	288.52	J/mol×K	618.94	Joback Method
dvisc	0.0001995	Pa×s	448.05	Joback Method
dvisc	0.0003442	Pa×s	413.85	Joback Method
dvisc	0.0006553	Pa×s	379.65	Joback Method
dvisc	0.0014170	Pa×s	345.45	Joback Method
dvisc	0.0036303	Pa×s	311.25	Joback Method
dvisc	0.0117321	Pa×s	277.05	Joback Method
dvisc	0.0527584	Pa×s	242.85	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.87890e+01
Coeff. B	-5.15009e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	343.82
Temperature range (K), max.	447.58

Sources

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=C56539663&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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