3-METHOXY-3-METHYL-1-BUTANOL

Other names: 1-Butanol, 3-methoxy-3-methyl-
3-Methyl-3-methoxy-1-butanol
3-methoxy-3-methylbutan-1-ol
3-methoxy-3-methylbutanol
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]: 118.18
CAS: 56539-66-3

Physical Properties

Property code	Value	Unit	Source
hf	-473.56	kJ/mol	Cheméo Relay (1.0)
hfus	9.16	kJ/mol	Joback Method
hvap	58.48	kJ/mol	Cheméo Relay (1.0)
log10ws	0.64		Cheméo Relay (1.0)
logp	0.794		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
ripol	1434.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	443.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.93	J/mol×K	448.05	Joback Method
cpg	243.25	J/mol×K	476.53	Joback Method
cpg	253.13	J/mol×K	505.01	Joback Method
cpg	262.58	J/mol×K	533.49	Joback Method
cpg	271.62	J/mol×K	561.97	Joback Method
cpg	280.27	J/mol×K	590.46	Joback Method
cpg	288.52	J/mol×K	618.94	Joback Method
dvisc	0.0527584	Pa×s	242.85	Joback Method

dvisc	0.0117321	Pa×s	277.05	Joback Method
dvisc	0.0036303	Pa×s	311.25	Joback Method
dvisc	0.0014170	Pa×s	345.45	Joback Method
dvisc	0.0006553	Pa×s	379.65	Joback Method
dvisc	0.0003442	Pa×s	413.85	Joback Method
dvisc	0.0001995	Pa×s	448.05	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56539663&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature