3-Methoxy-1-butyl acetate

Other names:	3-Methoxy-1-butanol, acetate
	3-Methoxybutylester kyseliny octove
	3-methoxy-n-butyl acetate
	3-methoxybutyl acetate
	Acetic acid, 3-methoxybutyl ester
	Butoxyl
	UN 2708
	acetic acid 3-methoxybutyl ester
Inchi:	InChI=1S/C7H14O3/c1-6(9-3)4-5-10-7(2)8/h6H,4-5H2,1-3H3
InchiKey:	QMYGFTJCQFEDST-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	COC(C)CCOC(C)=O
Mol. weight [g/mol]:	146.19

Physical Properties

Property code	Value	Unit	Source
af	0.4820		Cheméo Relay (1.0)
hf	-633.44	kJ/mol	Cheméo Relay (1.0)
hfus	14.34	kJ/mol	Joback Method
hvap	49.43	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	0.15		Cheméo Relay (1.0)
logp	0.974		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	442.04	K	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
tc	607.04	K	Cheméo Relay (1.0)
tf	215.14	K	Cheméo Relay (1.0)
vc	0.457	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.88	J/mol×K	457.83	Joback Method
cpg	324.24	J/mol×K	637.68	Joback Method
cpg	314.74	J/mol×K	607.71	Joback Method
cpg	304.87	J/mol×K	577.73	Joback Method
cpg	294.65	J/mol×K	547.76	Joback Method
cpg	284.07	J/mol×K	517.78	Joback Method
cpg	273.14	J/mol×K	487.81	Joback Method
dvisc	0.0002170	Pa×s	457.83	Joback Method
dvisc	0.0034521	Pa×s	248.04	Joback Method
dvisc	0.0016371	Pa×s	283.00	Joback Method
dvisc	0.0009148	Pa×s	317.97	Joback Method
dvisc	0.0005737	Pa×s	352.94	Joback Method
dvisc	0.0003913	Pa×s	387.90	Joback Method
dvisc	0.0002844	Pa×s	422.87	Joback Method
pvap	46.26	kPa	416.58	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
pvap	1.22	kPa	328.91	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
pvap	101.33	kPa	442.04	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
pvap	61.99	kPa	426.02	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate

pvap	3.52	kPa	350.20	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
pvap	20.93	kPa	393.70	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
pvap	10.00	kPa	374.40	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
pvap	6.43	kPa	363.37	Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate
rhol	975.30	kg/m3	273.15	Below the room temperature measurements of CO2 solubilities in six physical absorbents
rhol	965.30	kg/m3	283.15	Below the room temperature measurements of CO2 solubilities in six physical absorbents

Sources

Cheméo Relay (1.0):	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4435534&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubilities of Sulfuryl Fluoride in 2-Butoxyethyl Acetate, 3-Methoxybutyl Acetate, 2-Methoxyethyl Acetate, 1-Methoxy-2-propyl Acetate, and 2-(2-Ethoxyethoxy)ethyl Acetate:	https://www.doi.org/10.1021/acs.jced.8b00224
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	

Solubilities of carbon dioxide in 2-methoxyethyl acetate, 1-methoxy-2-propyl acetate and 3-methoxybutyl acetate: https://www.doi.org/10.1016/j.jct.2014.01.019

Below the room temperature measurements of CO2 solubilities in six physical absorbents: https://www.doi.org/10.1016/j.jct.2018.03.009

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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume