3-METHOXYBUTYRALDEHYDE DIMETHYL ACETAL

Other names: 1,1,3-Trimethoxybutane
3-Methoxybutyraldehyde dimethyl acetal
Butyraldehyde, 3-methoxy-, dimethyl acetal

Inchi: InChI=1S/C7H16O3/c1-6(8-2)5-7(9-3)10-4/h6-7H,5H2,1-4H3

InchiKey: OMAKZNALRADTRX-UHFFFAOYSA-N

Formula: C7H16O3

SMILES: COC(C)CC(OC)OC

Mol. weight [g/mol]: 148.20

Physical Properties

Property code	Value	Unit	Source
hfus	10.40	kJ/mol	Joback Method
hvap	46.14	kJ/mol	Cheméo Relay (1.0)
ie	9.11	eV	Cheméo Relay (1.0)
logp	1.030		Crippen Method
mcvol	127.100	ml/mol	McGowan Method
rinpol	877.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	430.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.11	J/mol×K	425.94	Joback Method
cpg	332.64	J/mol×K	598.37	Joback Method
cpg	322.29	J/mol×K	569.63	Joback Method
cpg	311.63	J/mol×K	540.90	Joback Method
cpg	300.66	J/mol×K	512.16	Joback Method
cpg	289.41	J/mol×K	483.42	Joback Method
cpg	277.89	J/mol×K	454.68	Joback Method
dvisc	0.0005052	Pa×s	315.64	Joback Method
dvisc	0.0001587	Pa×s	425.94	Joback Method
dvisc	0.0002170	Pa×s	389.17	Joback Method

dvisc	0.0003168	Pa×s	352.41	Joback Method
dvisc	0.0055798	Pa×s	205.34	Joback Method
dvisc	0.0009109	Pa×s	278.87	Joback Method
dvisc	0.0019646	Pa×s	242.11	Joback Method

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10138893&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature