

1-Methyl-2-methoxyethyl butyrate

Inchi:	InChI=1S/C8H16O3/c1-4-5-8(9)11-7(2)6-10-3/h7H,4-6H2,1-3H3
InchiKey:	UJXNFMNODANVBL-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCC(=O)OC(C)COC
Mol. weight [g/mol]:	160.21

Physical Properties

Property code	Value	Unit	Source
gf	-324.88	kJ/mol	Joback Method
hf	-590.75	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	44.58	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.365		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1017.00		NIST Webbook
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tb	480.71	K	Joback Method
tc	658.97	K	Joback Method
tf	259.31	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.01	J/mol×K	480.71	Joback Method
cpg	361.90	J/mol×K	629.26	Joback Method
cpg	351.15	J/mol×K	599.55	Joback Method
cpg	339.98	J/mol×K	569.84	Joback Method
cpg	328.40	J/mol×K	540.13	Joback Method
cpg	316.41	J/mol×K	510.42	Joback Method
cpg	372.23	J/mol×K	658.97	Joback Method
dvisc	0.0002029	Pa×s	480.71	Joback Method

dvisc	0.0002672	Pa×s	443.81	Joback Method
dvisc	0.0003699	Pa×s	406.91	Joback Method
dvisc	0.0005464	Pa×s	370.01	Joback Method
dvisc	0.0008800	Pa×s	333.11	Joback Method
dvisc	0.0015960	Pa×s	296.21	Joback Method
dvisc	0.0034290	Pa×s	259.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540084&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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