1-Methyl-2-methoxyethyl pentanoate

Inchi: InChI=1S/C9H18O3/c1-4-5-6-9(10)12-8(2)7-11-3/h8H,4-7H2,1-3H3
InchiKey: IOQOAKZXOSLXED-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCCCC(=O)OC(C)COC
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-316.46	kJ/mol	Joback Method
hf	-611.39	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.755		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1114.00		NIST Webbook
tb	503.59	K	Joback Method
tc	680.25	K	Joback Method
tf	270.58	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.25	J/mol×K	503.59	Joback Method
cpg	361.64	J/mol×K	533.03	Joback Method
cpg	374.58	J/mol×K	562.48	Joback Method
cpg	387.05	J/mol×K	591.92	Joback Method
cpg	399.06	J/mol×K	621.36	Joback Method
cpg	410.59	J/mol×K	650.81	Joback Method
cpg	421.65	J/mol×K	680.25	Joback Method
dvisc	0.0033518	Pa×s	270.58	Joback Method
dvisc	0.0015333	Pa×s	309.41	Joback Method

dvisc	0.0008351	Pa×s	348.25	Joback Method
dvisc	0.0005138	Pa×s	387.09	Joback Method
dvisc	0.0003454	Pa×s	425.92	Joback Method
dvisc	0.0002481	Pa×s	464.75	Joback Method
dvisc	0.0001875	Pa×s	503.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540217&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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