1-Methyl-2-methoxyethyl heptanoate

Inchi: InChI=1S/C11H22O3/c1-4-5-6-7-8-11(12)14-10(2)9-13-3/h10H,4-9H2,1-3H3
InchiKey: OXTYHPWTLWCXNE-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: CCCCCCC(=O)OC(C)COC
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	-299.62	kJ/mol	Joback Method
hf	-652.67	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	51.26	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.535		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1307.00		NIST Webbook
tb	549.35	K	Joback Method
tc	723.04	K	Joback Method
tf	293.12	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.54	J/mol×K	549.35	Joback Method
cpg	457.61	J/mol×K	578.30	Joback Method
cpg	472.13	J/mol×K	607.25	Joback Method
cpg	486.07	J/mol×K	636.19	Joback Method
cpg	499.46	J/mol×K	665.14	Joback Method
cpg	512.28	J/mol×K	694.09	Joback Method
cpg	524.54	J/mol×K	723.04	Joback Method
dvisc	0.0030774	Pa×s	293.12	Joback Method
dvisc	0.0013647	Pa×s	335.82	Joback Method

dvisc	0.0007270	Pa×s	378.53	Joback Method
dvisc	0.0004401	Pa×s	421.24	Joback Method
dvisc	0.0002922	Pa×s	463.94	Joback Method
dvisc	0.0002079	Pa×s	506.65	Joback Method
dvisc	0.0001559	Pa×s	549.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540148&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