1-(1-Methoxypropan-2-yloxy)propan-2-yl nonanoate

Inchi: InChI=1S/C16H32O4/c1-5-6-7-8-9-10-11-16(17)20-15(3)13-19-14(2)12-18-4/h14-15H,5-1

InchiKey: BRPKGDJYNHVTCZ-UHFFFAOYSA-N

Formula: C16H32O4

SMILES: CCCCCCCCC(=O)OC(C)COC(C)COC

Mol. weight [g/mol]: 288.42

Physical Properties

Property code	Value	Unit	Source
gf	-364.96	kJ/mol	Joback Method
hf	-893.37	kJ/mol	Joback Method
hfus	35.31	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.720		Crippen Method
mcvol	255.480	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	1799.00		NIST Webbook
tb	685.73	K	Joback Method
tc	858.63	K	Joback Method
tf	356.70	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.50	J/mol×K	685.73	Joback Method
cpg	820.13	J/mol×K	829.81	Joback Method
cpg	805.43	J/mol×K	800.99	Joback Method
cpg	789.92	J/mol×K	772.18	Joback Method
cpg	773.59	J/mol×K	743.36	Joback Method
cpg	756.45	J/mol×K	714.55	Joback Method
cpg	834.01	J/mol×K	858.63	Joback Method
dvisc	0.0000622	Pa×s	685.73	Joback Method
dvisc	0.0000854	Pa×s	630.89	Joback Method

dvisc	0.0001247	Pa×s	576.05	Joback Method
dvisc	0.0001970	Pa×s	521.22	Joback Method
dvisc	0.0003467	Pa×s	466.38	Joback Method
dvisc	0.0007092	Pa×s	411.54	Joback Method
dvisc	0.0018079	Pa×s	356.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378259&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