Nonanoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C15H30O3/c1-4-5-6-7-8-9-10-15(16)18-13-14(2)11-12-17-3/h14H,4-13H2,1-3H
InchiKey: VOBXHCAGLYWYDA-UHFFFAOYSA-N
Formula: C15H30O3
SMILES: CCCCCCCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]: 258.40

Physical Properties

Property code	Value	Unit	Source
gf	-265.94	kJ/mol	Joback Method
hf	-735.23	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.953		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	1770.00		NIST Webbook
tb	640.87	K	Joback Method
tc	811.05	K	Joback Method
tf	338.20	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.33	J/mol×K	640.87	Joback Method
cpg	668.79	J/mol×K	669.23	Joback Method
cpg	685.51	J/mol×K	697.60	Joback Method
cpg	701.51	J/mol×K	725.96	Joback Method
cpg	716.78	J/mol×K	754.32	Joback Method
cpg	731.33	J/mol×K	782.69	Joback Method
cpg	745.18	J/mol×K	811.05	Joback Method
dvisc	0.0023029	Pa×s	338.20	Joback Method
dvisc	0.0009707	Pa×s	388.64	Joback Method

dvisc	0.0004990	Pa×s	439.09	Joback Method
dvisc	0.0002942	Pa×s	489.53	Joback Method
dvisc	0.0001915	Pa×s	539.98	Joback Method
dvisc	0.0001341	Pa×s	590.42	Joback Method
dvisc	0.0000993	Pa×s	640.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360668&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