3-Methoxybutyl nonanoate

Inchi: InChI=1S/C14H28O3/c1-4-5-6-7-8-9-10-14(15)17-12-11-13(2)16-3/h13H,4-12H2,1-3H3
InchiKey: QUGPMGAIYMDVFN-UHFFFAOYSA-N
Formula: C14H28O3
SMILES: CCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]: 244.37

Physical Properties

Property code	Value	Unit	Source
gf	-274.36	kJ/mol	Joback Method
hf	-714.59	kJ/mol	Joback Method
hfus	32.47	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.705		Crippen Method
mcvol	221.430	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	1625.00		NIST Webbook
tb	617.99	K	Joback Method
tc	788.61	K	Joback Method
tf	326.93	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.87	J/mol×K	617.99	Joback Method
cpg	613.82	J/mol×K	646.43	Joback Method
cpg	630.08	J/mol×K	674.86	Joback Method
cpg	645.65	J/mol×K	703.30	Joback Method
cpg	660.54	J/mol×K	731.74	Joback Method
cpg	674.74	J/mol×K	760.17	Joback Method
cpg	688.27	J/mol×K	788.61	Joback Method
dvisc	0.0025063	Pa×s	326.93	Joback Method
dvisc	0.0010686	Pa×s	375.44	Joback Method

dvisc	0.0005538	Pa×s	423.95	Joback Method
dvisc	0.0003285	Pa×s	472.46	Joback Method
dvisc	0.0002147	Pa×s	520.97	Joback Method
dvisc	0.0001509	Pa×s	569.48	Joback Method
dvisc	0.0001121	Pa×s	617.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540995&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