3-Methoxybutyl undecanoate

Inchi: InChI=1S/C16H32O3/c1-4-5-6-7-8-9-10-11-12-16(17)19-14-13-15(2)18-3/h15H,4-14H2,1
InchiKey: OZVNZRAZEMUUFA-UHFFFAOYSA-N
Formula: C16H32O3
SMILES: CCCCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]: 272.42

Physical Properties

Property code	Value	Unit	Source
gf	-257.52	kJ/mol	Joback Method
hf	-755.87	kJ/mol	Joback Method
hfus	37.65	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.485		Crippen Method
mcvol	249.610	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	1823.00		NIST Webbook
tb	663.75	K	Joback Method
tc	833.87	K	Joback Method
tf	349.47	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.13	J/mol×K	663.75	Joback Method
cpg	789.07	J/mol×K	805.52	Joback Method
cpg	774.21	J/mol×K	777.17	Joback Method
cpg	758.59	J/mol×K	748.81	Joback Method
cpg	742.21	J/mol×K	720.46	Joback Method
cpg	725.06	J/mol×K	692.10	Joback Method
cpg	803.19	J/mol×K	833.87	Joback Method
dvisc	0.0000876	Pa×s	663.75	Joback Method
dvisc	0.0001186	Pa×s	611.37	Joback Method

dvisc	0.0001699	Pa×s	558.99	Joback Method
dvisc	0.0002622	Pa×s	506.61	Joback Method
dvisc	0.0004471	Pa×s	454.23	Joback Method
dvisc	0.0008764	Pa×s	401.85	Joback Method
dvisc	0.0021019	Pa×s	349.47	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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