1-(1-Methoxypropan-2-yloxy)propan-2-yl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C16H32O4/c1-12(9-16(4,5)6)8-15(17)20-14(3)11-19-13(2)10-18-7/h12-14H,8-1

InchiKey: NFVCTDXZJVLHNR-UHFFFAOYSA-N

Formula: C16H32O4

SMILES: COCC(C)OCC(C)OC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 288.42

Physical Properties

Property code	Value	Unit	Source
gf	-364.56	kJ/mol	Joback Method
hf	-907.40	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.432		Crippen Method
mcvol	255.480	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	682.06	K	Joback Method
tc	863.43	K	Joback Method
tf	344.12	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.11	J/mol×K	682.06	Joback Method
cpg	759.79	J/mol×K	712.29	Joback Method
cpg	777.53	J/mol×K	742.52	Joback Method
cpg	794.34	J/mol×K	772.74	Joback Method
cpg	810.24	J/mol×K	802.97	Joback Method
cpg	825.24	J/mol×K	833.20	Joback Method
cpg	839.35	J/mol×K	863.43	Joback Method
dvisc	0.0026908	Pa×s	344.12	Joback Method

dvisc	0.0008626	Pa×s	400.44	Joback Method
dvisc	0.0003661	Pa×s	456.77	Joback Method
dvisc	0.0001875	Pa×s	513.09	Joback Method
dvisc	0.0001096	Pa×s	569.41	Joback Method
dvisc	0.0000706	Pa×s	625.74	Joback Method
dvisc	0.0000489	Pa×s	682.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378245&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