2-(2-Methoxyethoxy)ethyl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C14H28O4/c1-12(11-14(2,3)4)10-13(15)18-9-8-17-7-6-16-5/h12H,6-11H2,1-5H

InchiKey: MCOMGHQPFGSTRN-UHFFFAOYSA-N

Formula: C14H28O4

SMILES: COCCOCCOC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	-376.52	kJ/mol	Joback Method
hf	-855.56	kJ/mol	Joback Method
hfus	26.24	kJ/mol	Joback Method
hvap	59.05	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.655		Crippen Method
mcvol	227.300	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	1633.00		NIST Webbook
rinpol	1633.00		NIST Webbook
tb	637.18	K	Joback Method
tc	815.02	K	Joback Method
tf	351.58	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.06	J/mol×K	637.18	Joback Method
cpg	646.39	J/mol×K	666.82	Joback Method
cpg	662.91	J/mol×K	696.46	Joback Method
cpg	678.64	J/mol×K	726.10	Joback Method
cpg	693.59	J/mol×K	755.74	Joback Method
cpg	707.77	J/mol×K	785.38	Joback Method
cpg	721.18	J/mol×K	815.02	Joback Method
dvisc	0.0018797	Pa×s	351.58	Joback Method

dvisc	0.0007998	Pa×s	399.18	Joback Method
dvisc	0.0004082	Pa×s	446.78	Joback Method
dvisc	0.0002372	Pa×s	494.38	Joback Method
dvisc	0.0001516	Pa×s	541.98	Joback Method
dvisc	0.0001042	Pa×s	589.58	Joback Method
dvisc	0.0000757	Pa×s	637.18	Joback Method

Sources

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=U378246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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