

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

Inchi:	InChI=1S/C16H32O5/c1-14(13-16(2,3)4)12-15(17)21-11-10-20-9-8-19-7-6-18-5/h14H,6-
InchiKey:	JZLGNZRORRBHPC-UHFFFAOYSA-N
Formula:	C16H32O5
SMILES:	COCCOCCOCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	304.42

Physical Properties

Property code	Value	Unit	Source
gf	-464.68	kJ/mol	Joback Method
hf	-1029.06	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	65.91	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.672		Crippen Method
mvol	261.350	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	1905.00		NIST Webbook
tb	705.36	K	Joback Method
tc	882.53	K	Joback Method
tf	396.35	K	Joback Method
vc	0.993	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	771.05	J/molxK	705.36	Joback Method
cpg	788.91	J/molxK	734.89	Joback Method
cpg	805.87	J/molxK	764.42	Joback Method
cpg	821.95	J/molxK	793.94	Joback Method
cpg	837.15	J/molxK	823.47	Joback Method
cpg	851.47	J/molxK	853.00	Joback Method
cpg	864.91	J/molxK	882.53	Joback Method
dvisc	0.0009774	Paxs	396.35	Joback Method
dvisc	0.0004300	Paxs	447.85	Joback Method

dvisc	0.0002241	Paxs	499.35	Joback Method
dvisc	0.0001319	Paxs	550.86	Joback Method
dvisc	0.0000850	Paxs	602.36	Joback Method
dvisc	0.0000587	Paxs	653.86	Joback Method
dvisc	0.0000428	Paxs	705.36	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=U378258&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

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