1-tert-Butoxypropan-2-yl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C16H32O3/c1-12(10-15(3,4)5)9-14(17)19-13(2)11-18-16(6,7)8/h12-13H,9-11H

InchiKey: WOBCBGRPPLPSMU-UHFFFAOYSA-N

Formula: C16H32O3

SMILES: CC(CC(=O)OC(C)COC(C)(C)C)CC(C)(C)C

Mol. weight [g/mol]: 272.42

Physical Properties

Property code	Value	Unit	Source
gf	-254.28	kJ/mol	Joback Method
hf	-778.65	kJ/mol	Joback Method
hfus	19.30	kJ/mol	Joback Method
hvap	59.41	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.196		Crippen Method
mcvol	249.610	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	1527.00		NIST Webbook
rinpol	1527.00		NIST Webbook
tb	656.85	K	Joback Method
tc	843.52	K	Joback Method
tf	339.31	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.21	J/mol×K	656.85	Joback Method
cpg	731.60	J/mol×K	687.96	Joback Method
cpg	749.96	J/mol×K	719.07	Joback Method
cpg	767.31	J/mol×K	750.18	Joback Method
cpg	783.70	J/mol×K	781.30	Joback Method
cpg	799.16	J/mol×K	812.41	Joback Method
cpg	813.73	J/mol×K	843.52	Joback Method
dvisc	0.0035646	Pa×s	339.31	Joback Method

dvisc	0.0011413	Pa×s	392.23	Joback Method
dvisc	0.0004790	Pa×s	445.16	Joback Method
dvisc	0.0002418	Pa×s	498.08	Joback Method
dvisc	0.0001392	Pa×s	551.00	Joback Method
dvisc	0.0000883	Pa×s	603.93	Joback Method
dvisc	0.0000602	Pa×s	656.85	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=U378314&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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