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

Inchi: InChI=1S/C19H38O4/c1-8-9-10-21-13-16(3)22-14-17(4)23-18(20)11-15(2)12-19(5,6)7/h1

InchiKey: PGFMVCGDTBSNIV-UHFFFAOYSA-N

Formula: C19H38O4

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

Mol. weight [g/mol]: 330.50

Physical Properties

Property code	Value	Unit	Source
gf	-339.30	kJ/mol	Joback Method
hf	-969.32	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.602		Crippen Method
mcvol	297.750	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	1882.00		NIST Webbook
tb	750.70	K	Joback Method
tc	932.18	K	Joback Method
tf	377.93	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.52	J/mol×K	750.70	Joback Method
cpg	936.06	J/mol×K	780.95	Joback Method
cpg	954.54	J/mol×K	811.19	Joback Method
cpg	971.98	J/mol×K	841.44	Joback Method
cpg	988.40	J/mol×K	871.69	Joback Method
cpg	1003.82	J/mol×K	901.94	Joback Method
cpg	1018.26	J/mol×K	932.18	Joback Method
dvisc	0.0017382	Pa×s	377.93	Joback Method
dvisc	0.0005529	Pa×s	440.06	Joback Method

dvisc	0.0002335	Pa×s	502.19	Joback Method
dvisc	0.0001192	Pa×s	564.32	Joback Method
dvisc	0.0000696	Pa×s	626.44	Joback Method
dvisc	0.0000447	Pa×s	688.57	Joback Method
dvisc	0.0000309	Pa×s	750.70	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378243&Units=SI

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