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

Inchi: InChI=1S/C16H32O3/c1-7-8-9-18-12-14(3)19-15(17)10-13(2)11-16(4,5)6/h13-14H,7-12H
InchiKey: NOYVLOUNQXVHIM-UHFFFAOYSA-N
Formula: C16H32O3
SMILES: CCCCOCC(C)OC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 272.42

Physical Properties

Property code	Value	Unit	Source
gf	-257.12	kJ/mol	Joback Method
hf	-769.90	kJ/mol	Joback Method
hfus	26.71	kJ/mol	Joback Method
hvap	60.70	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	4.197		Crippen Method
mcvol	249.610	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	660.08	K	Joback Method
tc	839.01	K	Joback Method
tf	336.89	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.86	J/mol×K	660.08	Joback Method
cpg	728.59	J/mol×K	689.90	Joback Method
cpg	746.42	J/mol×K	719.72	Joback Method
cpg	763.36	J/mol×K	749.54	Joback Method
cpg	779.43	J/mol×K	779.37	Joback Method
cpg	794.64	J/mol×K	809.19	Joback Method
cpg	809.04	J/mol×K	839.01	Joback Method
dvisc	0.0031635	Pa×s	336.89	Joback Method

dvisc	0.0010813	Pa×s	390.75	Joback Method
dvisc	0.0004794	Pa×s	444.62	Joback Method
dvisc	0.0002534	Pa×s	498.49	Joback Method
dvisc	0.0001517	Pa×s	552.35	Joback Method
dvisc	0.0000994	Pa×s	606.22	Joback Method
dvisc	0.0000699	Pa×s	660.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378244&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

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