2,2,4-Trimethyl-1,3-pentanediol diisobutyrate

Other names:	Propanoic acid, 2-methyl-, 2,2-dimethyl-1-(1-methylethyl)-1,3-propanediyl ester
	1,3-Pentanediol, 2,2,4-trimethyl-, diisobutyrate
	Kodaflex txib
	Isobutyric acid, 1-isopropyl-2,2-dimethyltrimethylene ester
	2,2,4-Trimethylpentanediol-1,3-diisobutyrate
	Txib
	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate
Inchi:	InChI=1S/C16H30O4/c1-10(2)13(20-15(18)12(5)6)16(7,8)9-19-14(17)11(3)4/h10-13H,9H
InchiKey:	OMVSWZDEEGIJJI-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CC(C)C(=O)OCC(C)(C)C(OC(=O)C(C)C)C(C)C
Mol. weight [g/mol]:	286.41
CAS:	6846-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-390.92	kJ/mol	Joback Method
hf	-893.04	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	66.67	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.436		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1587.50		NIST Webbook
rinpol	1587.50		NIST Webbook
tb	713.07	K	Joback Method
tc	904.59	K	Joback Method
tf	356.82	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.61	J/mol×K	713.07	Joback Method
cpg	816.90	J/mol×K	872.67	Joback Method
cpg	802.99	J/mol×K	840.75	Joback Method
cpg	788.13	J/mol×K	808.83	Joback Method
cpg	772.29	J/mol×K	776.91	Joback Method
cpg	755.46	J/mol×K	744.99	Joback Method
cpg	829.89	J/mol×K	904.59	Joback Method
dvisc	0.0000565	Pa×s	713.07	Joback Method
dvisc	0.0000822	Pa×s	653.70	Joback Method
dvisc	0.0001289	Pa×s	594.32	Joback Method
dvisc	0.0002234	Pa×s	534.95	Joback Method
dvisc	0.0004442	Pa×s	475.57	Joback Method
dvisc	0.0010748	Pa×s	416.20	Joback Method
dvisc	0.0034893	Pa×s	356.82	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=C6846500&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