2,4,4-trimethyl pentyl 3,5,5-trimethyl hexanoate

Inchi: InChI=1S/C17H34O2/c1-13(10-16(3,4)5)9-15(18)19-12-14(2)11-17(6,7)8/h13-14H,9-12H

InchiKey: FINRZAGSLZQHHT-UHFFFAOYSA-N

Formula: C17H34O2

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

Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	-140.86	kJ/mol	Joback Method
hf	-667.07	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	59.22	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	5.064		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
ripol	1706.00		NIST Webbook
ripol	1706.00		NIST Webbook
tb	657.31	K	Joback Method
tc	843.23	K	Joback Method
tf	328.35	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.56	J/mol×K	657.31	Joback Method
cpg	757.68	J/mol×K	688.30	Joback Method
cpg	776.71	J/mol×K	719.28	Joback Method
cpg	794.71	J/mol×K	750.27	Joback Method
cpg	811.72	J/mol×K	781.25	Joback Method
cpg	827.79	J/mol×K	812.24	Joback Method
cpg	842.98	J/mol×K	843.23	Joback Method
dvisc	0.0051939	Pa×s	328.35	Joback Method

dvisc	0.0015092	Pa×s	383.18	Joback Method
dvisc	0.0005975	Pa×s	438.00	Joback Method
dvisc	0.0002908	Pa×s	492.83	Joback Method
dvisc	0.0001634	Pa×s	547.66	Joback Method
dvisc	0.0001020	Pa×s	602.48	Joback Method
dvisc	0.0000689	Pa×s	657.31	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=R328022&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume