METHYL 2,6,10-TRIMETHYLTRIDECANOATE

Other names: Methyl hexadecanoate (isoprenoid)
Tridecanoic acid, 2,6,10-trimethyl, methyl ester
Inchi: InChI=1S/C17H34O2/c1-6-9-14(2)10-7-11-15(3)12-8-13-16(4)17(18)19-5/h14-16H,6-13H
InchiKey: AJQKJNYTUWSMBZ-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CCCC(C)CCCC(C)CCCC(C)C(=O)OC
Mol. weight [g/mol]: 270.46

Physical Properties

Property code	Value	Unit	Source
af	0.7206		Cheméo Relay (1.0)
gf	-148.98	kJ/mol	Joback Method
hf	-746.29	kJ/mol	Cheméo Relay (1.0)
hfus	32.00	kJ/mol	Joback Method
hvap	83.21	kJ/mol	Cheméo Relay (1.0)
logp	5.208		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
tb	537.37	K	Cheméo Relay (1.0)
tc	727.11	K	Cheméo Relay (1.0)
tf	232.38	K	Cheméo Relay (1.0)
vc	0.945	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.46	J/mol×K	663.33	Joback Method
cpg	752.60	J/mol×K	692.33	Joback Method
cpg	770.87	J/mol×K	721.32	Joback Method
cpg	788.28	J/mol×K	750.32	Joback Method
cpg	804.86	J/mol×K	779.31	Joback Method
cpg	820.61	J/mol×K	808.31	Joback Method
cpg	835.57	J/mol×K	837.31	Joback Method
dvisc	0.0054749	Pa×s	308.51	Joback Method

dvisc	0.0015723	Pa×s	367.65	Joback Method
dvisc	0.0006381	Pa×s	426.78	Joback Method
dvisc	0.0003225	Pa×s	485.92	Joback Method
dvisc	0.0001890	Pa×s	545.06	Joback Method
dvisc	0.0001230	Pa×s	604.19	Joback Method
dvisc	0.0000864	Pa×s	663.33	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U131722&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume