Dimethylmalonic acid, hexadecyl undecyl ester

Inchi: InChI=1S/C32H62O4/c1-5-7-9-11-13-15-16-17-18-19-21-23-25-27-29-36-31(34)32(3,4)3
InchiKey: LXGNOXCOSQGJGH-UHFFFAOYSA-N
Formula: C32H62O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 510.83

Physical Properties

Property code	Value	Unit	Source
gf	-246.44	kJ/mol	Joback Method
hf	-1202.16	kJ/mol	Joback Method
hfus	76.80	kJ/mol	Joback Method
hvap	103.84	kJ/mol	Joback Method
log10ws	-10.70		Crippen Method
logp	10.111		Crippen Method
mcvol	476.620	ml/mol	McGowan Method
pc	572.61	kPa	Joback Method
rinpol	3291.00		NIST Webbook
rinpol	3291.00		NIST Webbook
tb	1080.91	K	Joback Method
tc	1367.66	K	Joback Method
tf	597.14	K	Joback Method
vc	1.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.61	J/mol×K	1080.91	Joback Method
cpg	1762.24	J/mol×K	1128.70	Joback Method
cpg	1785.28	J/mol×K	1176.49	Joback Method
cpg	1805.94	J/mol×K	1224.29	Joback Method
cpg	1824.42	J/mol×K	1272.08	Joback Method
cpg	1840.92	J/mol×K	1319.87	Joback Method
cpg	1855.66	J/mol×K	1367.66	Joback Method
dvisc	0.0001538	Pa×s	597.14	Joback Method

dvisc	0.0000653	Pa×s	677.77	Joback Method
dvisc	0.0000333	Pa×s	758.40	Joback Method
dvisc	0.0000193	Pa×s	839.02	Joback Method
dvisc	0.0000123	Pa×s	919.65	Joback Method
dvisc	0.0000084	Pa×s	1000.28	Joback Method
dvisc	0.0000061	Pa×s	1080.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361785&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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