Dimethylmalonic acid, cis-4-methylcyclohexyl octadecyl ester

Inchi: InChI=1S/C30H56O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-25-33-28(31)30(3

InchiKey: IAAWYDLPNWOOFK-UHFFFAOYSA-N

Formula: C30H56O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-246.54	kJ/mol	Joback Method
hf	-1126.90	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	99.51	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	8.939		Crippen Method
mcvol	437.580	ml/mol	McGowan Method
pc	687.09	kPa	Joback Method
rinpol	3256.00		NIST Webbook
rinpol	3256.00		NIST Webbook
tb	1050.03	K	Joback Method
tc	1294.66	K	Joback Method
tf	577.74	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.25	J/mol×K	1050.03	Joback Method
cpg	1625.29	J/mol×K	1090.80	Joback Method
cpg	1644.13	J/mol×K	1131.57	Joback Method
cpg	1660.89	J/mol×K	1172.35	Joback Method
cpg	1675.69	J/mol×K	1213.12	Joback Method
cpg	1688.63	J/mol×K	1253.89	Joback Method
cpg	1699.83	J/mol×K	1294.66	Joback Method
dvisc	0.0002649	Pa×s	577.74	Joback Method

dvisc	0.0001157	Pa×s	656.46	Joback Method
dvisc	0.0000604	Pa×s	735.17	Joback Method
dvisc	0.0000357	Pa×s	813.88	Joback Method
dvisc	0.0000232	Pa×s	892.60	Joback Method
dvisc	0.0000161	Pa×s	971.31	Joback Method
dvisc	0.0000119	Pa×s	1050.03	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U363891&Units=SI

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