Dimethylmalonic acid, hexadecyl 3-phenylpropyl ester

Inchi: InChI=1S/C30H50O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-25-33-28(31)30(2,3)29(32
InchiKey: LXNZRRXLDWPSCD-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-150.87	kJ/mol	Joback Method
hf	-924.35	kJ/mol	Joback Method
hfus	65.66	kJ/mol	Joback Method
hvap	101.67	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	8.213		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	748.15	kPa	Joback Method
rinpol	3242.00		NIST Webbook
tb	1061.83	K	Joback Method
tc	1308.19	K	Joback Method
tf	601.02	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.51	J/mol×K	1061.83	Joback Method
cpg	1577.81	J/mol×K	1267.13	Joback Method
cpg	1564.65	J/mol×K	1226.07	Joback Method
cpg	1550.17	J/mol×K	1185.01	Joback Method
cpg	1534.24	J/mol×K	1143.95	Joback Method
cpg	1516.73	J/mol×K	1102.89	Joback Method
cpg	1589.78	J/mol×K	1308.19	Joback Method
dvisc	0.0000088	Pa×s	1061.83	Joback Method
dvisc	0.0000120	Pa×s	985.03	Joback Method

dvisc	0.0000171	Pa×s	908.23	Joback Method
dvisc	0.0000261	Pa×s	831.42	Joback Method
dvisc	0.0000433	Pa×s	754.62	Joback Method
dvisc	0.0000807	Pa×s	677.82	Joback Method
dvisc	0.0001763	Pa×s	601.02	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=U361844&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