Dimethylmalonic acid, hexadecyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C27H52O4/c1-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-30-25(28)27(5,6)
InchiKey: FGOALVWKTQAWFY-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-293.42	kJ/mol	Joback Method
hf	-1109.52	kJ/mol	Joback Method
hfus	56.80	kJ/mol	Joback Method
hvap	91.94	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	8.015		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	737.22	kPa	Joback Method
rinpol	2756.00		NIST Webbook
tb	965.63	K	Joback Method
tc	1186.37	K	Joback Method
tf	510.79	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.02	J/mol×K	965.63	Joback Method
cpg	1431.21	J/mol×K	1002.42	Joback Method
cpg	1450.77	J/mol×K	1039.21	Joback Method
cpg	1468.78	J/mol×K	1076.00	Joback Method
cpg	1485.31	J/mol×K	1112.79	Joback Method
cpg	1500.44	J/mol×K	1149.58	Joback Method
cpg	1514.25	J/mol×K	1186.37	Joback Method
dvisc	0.0004279	Pa×s	510.79	Joback Method
dvisc	0.0001593	Pa×s	586.60	Joback Method

dvisc	0.0000744	Pa×s	662.40	Joback Method
dvisc	0.0000406	Pa×s	738.21	Joback Method
dvisc	0.0000248	Pa×s	814.02	Joback Method
dvisc	0.0000165	Pa×s	889.82	Joback Method
dvisc	0.0000117	Pa×s	965.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361801&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