Dimethylmalonic acid, octyl tetradecyl ester

Inchi: InChI=1S/C27H52O4/c1-5-7-9-11-13-14-15-16-17-18-20-22-24-31-26(29)27(3,4)25(28)3
InchiKey: KLIVXHJXRMSSGP-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-288.54	kJ/mol	Joback Method
hf	-1098.96	kJ/mol	Joback Method
hfus	63.85	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.161		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	2785.00		NIST Webbook
rinpol	2785.00		NIST Webbook
tb	966.51	K	Joback Method
tc	1190.06	K	Joback Method
tf	540.79	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.34	J/mol×K	966.51	Joback Method
cpg	1501.45	J/mol×K	1152.80	Joback Method
cpg	1486.00	J/mol×K	1115.54	Joback Method
cpg	1469.14	J/mol×K	1078.28	Joback Method
cpg	1450.80	J/mol×K	1041.03	Joback Method
cpg	1430.89	J/mol×K	1003.77	Joback Method
cpg	1515.58	J/mol×K	1190.06	Joback Method
dvisc	0.0000141	Pa×s	966.51	Joback Method

dvisc	0.0000192	Pa×s	895.56	Joback Method
dvisc	0.0000278	Pa×s	824.60	Joback Method
dvisc	0.0000431	Pa×s	753.65	Joback Method
dvisc	0.0000730	Pa×s	682.70	Joback Method
dvisc	0.0001400	Pa×s	611.74	Joback Method
dvisc	0.0003183	Pa×s	540.79	Joback Method

Sources

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=U361681&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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