Dimethylmalonic acid, hexadecyl 4-octyl ester

Inchi: InChI=1S/C29H56O4/c1-6-9-11-12-13-14-15-16-17-18-19-20-21-22-25-32-27(30)29(4,5)
InchiKey: QJICPZQJSTZTHS-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CCC)CCCC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-274.14	kJ/mol	Joback Method
hf	-1145.52	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	96.78	kJ/mol	Joback Method
log10ws	-9.56		Crippen Method
logp	8.939		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	663.23	kPa	Joback Method
rinpol	2859.00		NIST Webbook
tb	1011.83	K	Joback Method
tc	1253.72	K	Joback Method
tf	548.33	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.55	J/mol×K	1011.83	Joback Method
cpg	1634.74	J/mol×K	1213.40	Joback Method
cpg	1619.12	J/mol×K	1173.09	Joback Method
cpg	1601.90	J/mol×K	1132.77	Joback Method
cpg	1582.97	J/mol×K	1092.46	Joback Method
cpg	1562.22	J/mol×K	1052.14	Joback Method
cpg	1648.87	J/mol×K	1253.72	Joback Method
dvisc	0.0000092	Pa×s	1011.83	Joback Method
dvisc	0.0000128	Pa×s	934.58	Joback Method

dvisc	0.0000189	Pa×s	857.33	Joback Method
dvisc	0.0000303	Pa×s	780.08	Joback Method
dvisc	0.0000536	Pa×s	702.83	Joback Method
dvisc	0.0001093	Pa×s	625.58	Joback Method
dvisc	0.0002725	Pa×s	548.33	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=U361738&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

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