Dimethylmalonic acid, pentadecyl undecyl ester

Inchi: InChI=1S/C31H60O4/c1-5-7-9-11-13-15-16-17-18-20-22-24-26-28-35-30(33)31(3,4)29(3

InchiKey: PLTKNYVNXFNYGM-UHFFFAOYSA-N

Formula: C31H60O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCCCC

Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-254.86	kJ/mol	Joback Method
hf	-1181.52	kJ/mol	Joback Method
hfus	74.21	kJ/mol	Joback Method
hvap	101.62	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	9.721		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	599.85	kPa	Joback Method
rinpol	3188.00		NIST Webbook
rinpol	3188.00		NIST Webbook
tb	1058.03	K	Joback Method
tc	1328.97	K	Joback Method
tf	585.87	K	Joback Method
vc	1.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.57	J/mol×K	1058.03	Joback Method
cpg	1695.23	J/mol×K	1103.19	Joback Method
cpg	1717.54	J/mol×K	1148.34	Joback Method
cpg	1737.68	J/mol×K	1193.50	Joback Method
cpg	1755.80	J/mol×K	1238.66	Joback Method
cpg	1772.07	J/mol×K	1283.81	Joback Method
cpg	1786.66	J/mol×K	1328.97	Joback Method
dvisc	0.0001785	Pa×s	585.87	Joback Method

dvisc	0.0000763	Pa×s	664.56	Joback Method
dvisc	0.0000390	Pa×s	743.26	Joback Method
dvisc	0.0000227	Pa×s	821.95	Joback Method
dvisc	0.0000145	Pa×s	900.64	Joback Method
dvisc	0.0000100	Pa×s	979.34	Joback Method
dvisc	0.0000072	Pa×s	1058.03	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=U361776&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