Dimethylmalonic acid, heptadecyl 3-phenylpropyl ester

Inchi: InChI=1S/C31H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26-34-29(32)31(2,3)30
InchiKey: XVWYNLMXRBAEBY-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-142.45	kJ/mol	Joback Method
hf	-944.99	kJ/mol	Joback Method
hfus	68.25	kJ/mol	Joback Method
hvap	103.89	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.603		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	710.35	kPa	Joback Method
rinpol	3343.00		NIST Webbook
tb	1084.71	K	Joback Method
tc	1341.44	K	Joback Method
tf	612.29	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.76	J/mol×K	1084.71	Joback Method
cpg	1581.52	J/mol×K	1127.50	Joback Method
cpg	1599.47	J/mol×K	1170.29	Joback Method
cpg	1615.74	J/mol×K	1213.08	Joback Method
cpg	1630.49	J/mol×K	1255.86	Joback Method
cpg	1643.88	J/mol×K	1298.65	Joback Method
cpg	1656.06	J/mol×K	1341.44	Joback Method
dvisc	0.0001528	Pa×s	612.29	Joback Method
dvisc	0.0000694	Pa×s	691.03	Joback Method

dvisc	0.0000371	Pa×s	769.76	Joback Method
dvisc	0.0000222	Pa×s	848.50	Joback Method
dvisc	0.0000145	Pa×s	927.24	Joback Method
dvisc	0.0000102	Pa×s	1005.97	Joback Method
dvisc	0.0000075	Pa×s	1084.71	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=U361845&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