Dimethylmalonic acid, octadecyl 3-phenylpropyl ester

Inchi: InChI=1S/C32H54O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-27-35-30(33)32(2,3

InchiKey: RTQUSFKTROWEEG-UHFFFAOYSA-N

Formula: C32H54O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 502.77

Physical Properties

Property code	Value	Unit	Source
gf	-134.03	kJ/mol	Joback Method
hf	-965.63	kJ/mol	Joback Method
hfus	70.84	kJ/mol	Joback Method
hvap	106.12	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	8.993		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	675.35	kPa	Joback Method
rinpol	3452.00		NIST Webbook
rinpol	3452.00		NIST Webbook
tb	1107.59	K	Joback Method
tc	1376.17	K	Joback Method
tf	623.56	K	Joback Method
vc	1.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1626.31	J/mol×K	1107.59	Joback Method
cpg	1710.53	J/mol×K	1331.40	Joback Method
cpg	1696.86	J/mol×K	1286.64	Joback Method
cpg	1681.79	J/mol×K	1241.88	Joback Method
cpg	1665.13	J/mol×K	1197.12	Joback Method
cpg	1646.70	J/mol×K	1152.35	Joback Method
cpg	1722.97	J/mol×K	1376.17	Joback Method
dvisc	0.0000063	Pa×s	1107.59	Joback Method

dvisc	0.0000086	Pa×s	1026.92	Joback Method
dvisc	0.0000124	Pa×s	946.25	Joback Method
dvisc	0.0000189	Pa×s	865.57	Joback Method
dvisc	0.0000317	Pa×s	784.90	Joback Method
dvisc	0.0000596	Pa×s	704.23	Joback Method
dvisc	0.0001322	Pa×s	623.56	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=U361846&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