Diethylmalonic acid, 2,3-dimethylphenyl heptadecyl ester

Inchi: InChI=1S/C32H54O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-22-26-35-30(33)32(7

InchiKey: KRPQWEWSUUQONN-UHFFFAOYSA-N

Formula: C32H54O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 502.77

Physical Properties

Property code	Value	Unit	Source
gf	-153.29	kJ/mol	Joback Method
hf	-988.57	kJ/mol	Joback Method
hfus	70.06	kJ/mol	Joback Method
hvap	107.44	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.430		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	664.94	kPa	Joback Method
rinpol	3421.00		NIST Webbook
tb	1117.55	K	Joback Method
tc	1389.53	K	Joback Method
tf	648.60	K	Joback Method
vc	1.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1624.62	J/mol×K	1117.55	Joback Method
cpg	1644.46	J/mol×K	1162.88	Joback Method
cpg	1662.18	J/mol×K	1208.21	Joback Method
cpg	1677.93	J/mol×K	1253.54	Joback Method
cpg	1691.89	J/mol×K	1298.87	Joback Method
cpg	1704.21	J/mol×K	1344.20	Joback Method
cpg	1715.05	J/mol×K	1389.53	Joback Method
dvisc	0.0001041	Pa×s	648.60	Joback Method
dvisc	0.0000516	Pa×s	726.76	Joback Method

dvisc	0.0000293	Pa×s	804.92	Joback Method
dvisc	0.0000184	Pa×s	883.07	Joback Method
dvisc	0.0000125	Pa×s	961.23	Joback Method
dvisc	0.0000090	Pa×s	1039.39	Joback Method
dvisc	0.0000067	Pa×s	1117.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370578&Units=SI
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

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