Diethylmalonic acid, 2,3-dimethylphenyl octadecyl ester

Inchi: InChI=1S/C33H56O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-27-36-31(34)3

InchiKey: OBSBAGVOWWHCKG-UHFFFAOYSA-N

Formula: C33H56O4

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

Mol. weight [g/mol]: 516.80

Physical Properties

Property code	Value	Unit	Source
gf	-144.87	kJ/mol	Joback Method
hf	-1009.21	kJ/mol	Joback Method
hfus	72.65	kJ/mol	Joback Method
hvap	109.67	kJ/mol	Joback Method
log10ws	-10.99		Crippen Method
logp	9.820		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	633.20	kPa	Joback Method
rinpol	3548.00		NIST Webbook
tb	1140.43	K	Joback Method
tc	1426.12	K	Joback Method
tf	659.87	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1689.24	J/mol×K	1140.43	Joback Method
cpg	1770.39	J/mol×K	1378.51	Joback Method
cpg	1757.97	J/mol×K	1330.89	Joback Method
cpg	1743.85	J/mol×K	1283.28	Joback Method
cpg	1727.81	J/mol×K	1235.66	Joback Method
cpg	1709.68	J/mol×K	1188.05	Joback Method
cpg	1781.29	J/mol×K	1426.12	Joback Method
dvisc	0.0000057	Pa×s	1140.43	Joback Method
dvisc	0.0000076	Pa×s	1060.34	Joback Method

dvisc	0.0000106	Pa×s	980.24	Joback Method
dvisc	0.0000157	Pa×s	900.15	Joback Method
dvisc	0.0000252	Pa×s	820.06	Joback Method
dvisc	0.0000445	Pa×s	739.96	Joback Method
dvisc	0.0000905	Pa×s	659.87	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=U370579&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