Diethylmalonic acid, 2,3-dimethylphenyl hexadecyl ester

Inchi: InChI=1S/C31H52O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-25-34-29(32)31(7-2,8

InchiKey: QGESANMHSUGMMI-UHFFFAOYSA-N

Formula: C31H52O4

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

Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-161.71	kJ/mol	Joback Method
hf	-967.93	kJ/mol	Joback Method
hfus	67.47	kJ/mol	Joback Method
hvap	105.22	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.040		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	699.13	kPa	Joback Method
rinpol	3316.00		NIST Webbook
tb	1094.67	K	Joback Method
tc	1354.56	K	Joback Method
tf	637.33	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1560.25	J/mol×K	1094.67	Joback Method
cpg	1638.45	J/mol×K	1311.24	Joback Method
cpg	1626.20	J/mol×K	1267.93	Joback Method
cpg	1612.40	J/mol×K	1224.61	Joback Method
cpg	1596.89	J/mol×K	1181.30	Joback Method
cpg	1579.55	J/mol×K	1137.98	Joback Method
cpg	1649.27	J/mol×K	1354.56	Joback Method
dvisc	0.0000079	Pa×s	1094.67	Joback Method
dvisc	0.0000105	Pa×s	1018.45	Joback Method

dvisc	0.0000146	Pa×s	942.22	Joback Method
dvisc	0.0000215	Pa×s	866.00	Joback Method
dvisc	0.0000342	Pa×s	789.78	Joback Method
dvisc	0.0000598	Pa×s	713.55	Joback Method
dvisc	0.0001196	Pa×s	637.33	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=U370577&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