Diethylmalonic acid, hexadecyl 3-methylbenzyl ester

Inchi: InChI=1S/C31H52O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-24-34-29(32)31(6-2,7-
InchiKey: NXWMVNMCFNVXQP-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-152.08	kJ/mol	Joback Method
hf	-956.46	kJ/mol	Joback Method
hfus	67.86	kJ/mol	Joback Method
hvap	104.55	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.869		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	704.71	kPa	Joback Method
rinpol	3260.00		NIST Webbook
tb	1089.69	K	Joback Method
tc	1347.99	K	Joback Method
tf	624.81	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.03	J/mol×K	1089.69	Joback Method
cpg	1641.25	J/mol×K	1304.94	Joback Method
cpg	1628.42	J/mol×K	1261.89	Joback Method
cpg	1614.12	J/mol×K	1218.84	Joback Method
cpg	1598.22	J/mol×K	1175.79	Joback Method
cpg	1580.57	J/mol×K	1132.74	Joback Method
cpg	1652.77	J/mol×K	1347.99	Joback Method
dvisc	0.0000077	Pa×s	1089.69	Joback Method
dvisc	0.0000103	Pa×s	1012.21	Joback Method

dvisc	0.0000146	Pa×s	934.73	Joback Method
dvisc	0.0000219	Pa×s	857.25	Joback Method
dvisc	0.0000355	Pa×s	779.77	Joback Method
dvisc	0.0000642	Pa×s	702.29	Joback Method
dvisc	0.0001346	Pa×s	624.81	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=U369316&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