Diethylmalonic acid, 3-methylbenzyl octadecyl ester

Inchi: InChI=1S/C33H56O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-26-36-31(34)33
InchiKey: VMGZEHKIGZLICW-UHFFFAOYSA-N
Formula: C33H56O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]: 516.80

Physical Properties

Property code	Value	Unit	Source
gf	-135.24	kJ/mol	Joback Method
hf	-997.74	kJ/mol	Joback Method
hfus	73.04	kJ/mol	Joback Method
hvap	109.01	kJ/mol	Joback Method
log10ws	-10.77		Crippen Method
logp	9.649		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	638.01	kPa	Joback Method
rinpol	3524.00		NIST Webbook
tb	1135.45	K	Joback Method
tc	1419.29	K	Joback Method
tf	647.35	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1690.22	J/mol×K	1135.45	Joback Method
cpg	1710.99	J/mol×K	1182.76	Joback Method
cpg	1729.57	J/mol×K	1230.06	Joback Method
cpg	1746.15	J/mol×K	1277.37	Joback Method
cpg	1760.96	J/mol×K	1324.68	Joback Method
cpg	1774.20	J/mol×K	1371.99	Joback Method
cpg	1786.07	J/mol×K	1419.29	Joback Method
dvisc	0.0001012	Pa×s	647.35	Joback Method
dvisc	0.0000476	Pa×s	728.70	Joback Method

dvisc	0.0000260	Pa×s	810.05	Joback Method
dvisc	0.0000159	Pa×s	891.40	Joback Method
dvisc	0.0000105	Pa×s	972.75	Joback Method
dvisc	0.0000075	Pa×s	1054.10	Joback Method
dvisc	0.0000055	Pa×s	1135.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369318&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