Diethylmalonic acid, heptadecyl 3-methylphenyl ester

Inchi: InChI=1S/C31H52O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-34-29(32)31(6-

InchiKey: XWMBFTLXJVNJQH-UHFFFAOYSA-N

Formula: C31H52O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(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	-10.09		Crippen Method
logp	9.121		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	704.71	kPa	Joback Method
rinpol	3255.00		NIST Webbook
rinpol	3255.00		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	1580.57	J/mol×K	1132.74	Joback Method
cpg	1598.22	J/mol×K	1175.79	Joback Method
cpg	1614.12	J/mol×K	1218.84	Joback Method
cpg	1628.42	J/mol×K	1261.89	Joback Method
cpg	1641.25	J/mol×K	1304.94	Joback Method
cpg	1652.77	J/mol×K	1347.99	Joback Method
dvisc	0.0001346	Pa×s	624.81	Joback Method

dvisc	0.0000642	Pa×s	702.29	Joback Method
dvisc	0.0000355	Pa×s	779.77	Joback Method
dvisc	0.0000219	Pa×s	857.25	Joback Method
dvisc	0.0000146	Pa×s	934.73	Joback Method
dvisc	0.0000103	Pa×s	1012.21	Joback Method
dvisc	0.0000077	Pa×s	1089.69	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370025&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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