Diethylmalonic acid, 2,3-dimethylphenyl tetradecyl ester

Inchi: InChI=1S/C29H48O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-23-32-27(30)29(7-2,8-3)28

InchiKey: VSDKERXGMVSMIX-UHFFFAOYSA-N

Formula: C29H48O4

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

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-178.55	kJ/mol	Joback Method
hf	-926.65	kJ/mol	Joback Method
hfus	62.29	kJ/mol	Joback Method
hvap	100.76	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.260		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	775.91	kPa	Joback Method
rinpol	3116.00		NIST Webbook
tb	1048.91	K	Joback Method
tc	1288.99	K	Joback Method
tf	614.79	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.33	J/mol×K	1048.91	Joback Method
cpg	1450.73	J/mol×K	1088.92	Joback Method
cpg	1467.43	J/mol×K	1128.94	Joback Method
cpg	1482.51	J/mol×K	1168.95	Joback Method
cpg	1496.08	J/mol×K	1208.96	Joback Method
cpg	1508.23	J/mol×K	1248.97	Joback Method
cpg	1519.05	J/mol×K	1288.99	Joback Method
dvisc	0.0001568	Pa×s	614.79	Joback Method
dvisc	0.0000797	Pa×s	687.14	Joback Method

dvisc	0.0000461	Pa×s	759.50	Joback Method
dvisc	0.0000293	Pa×s	831.85	Joback Method
dvisc	0.0000201	Pa×s	904.20	Joback Method
dvisc	0.0000145	Pa×s	976.56	Joback Method
dvisc	0.0000110	Pa×s	1048.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370575&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