Diethylmalonic acid, 3-methylphenyl pentadecyl ester

Inchi: InChI=1S/C29H48O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-23-32-27(30)29(6-2,7-3)2

InchiKey: FDIPILODFWTMGN-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-168.92	kJ/mol	Joback Method
hf	-915.18	kJ/mol	Joback Method
hfus	62.68	kJ/mol	Joback Method
hvap	100.10	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.341		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	782.43	kPa	Joback Method
rinpol	3052.00		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	1043.93	K	Joback Method
tc	1282.64	K	Joback Method
tf	602.27	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.98	J/mol×K	1043.93	Joback Method
cpg	1451.55	J/mol×K	1083.72	Joback Method
cpg	1468.47	J/mol×K	1123.50	Joback Method
cpg	1483.84	J/mol×K	1163.29	Joback Method
cpg	1497.76	J/mol×K	1203.07	Joback Method
cpg	1510.33	J/mol×K	1242.86	Joback Method
cpg	1521.67	J/mol×K	1282.64	Joback Method
dvisc	0.0001776	Pa×s	602.27	Joback Method

dvisc	0.0000861	Pa×s	675.88	Joback Method
dvisc	0.0000482	Pa×s	749.49	Joback Method
dvisc	0.0000299	Pa×s	823.10	Joback Method
dvisc	0.0000201	Pa×s	896.71	Joback Method
dvisc	0.0000143	Pa×s	970.32	Joback Method
dvisc	0.0000107	Pa×s	1043.93	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=U370023&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