Diethylmalonic acid, hexadecyl 3-methylphenyl ester

Inchi: InChI=1S/C30H50O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-24-33-28(31)30(6-2,7-
InchiKey: PMPCUOICRDXDRU-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-160.50	kJ/mol	Joback Method
hf	-935.82	kJ/mol	Joback Method
hfus	65.27	kJ/mol	Joback Method
hvap	102.33	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.731		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	742.05	kPa	Joback Method
rinpol	3155.00		NIST Webbook
tb	1066.81	K	Joback Method
tc	1314.63	K	Joback Method
tf	613.54	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.84	J/mol×K	1066.81	Joback Method
cpg	1515.88	J/mol×K	1108.11	Joback Method
cpg	1533.14	J/mol×K	1149.42	Joback Method
cpg	1548.75	J/mol×K	1190.72	Joback Method
cpg	1562.85	J/mol×K	1232.02	Joback Method
cpg	1575.54	J/mol×K	1273.33	Joback Method
cpg	1586.95	J/mol×K	1314.63	Joback Method
dvisc	0.0001548	Pa×s	613.54	Joback Method
dvisc	0.0000745	Pa×s	689.08	Joback Method

dvisc	0.0000414	Pa×s	764.63	Joback Method
dvisc	0.0000256	Pa×s	840.17	Joback Method
dvisc	0.0000171	Pa×s	915.72	Joback Method
dvisc	0.0000122	Pa×s	991.26	Joback Method
dvisc	0.0000091	Pa×s	1066.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370024&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