Diethylmalonic acid, dodecyl 3-methylphenyl ester

Inchi: InChI=1S/C26H42O4/c1-5-8-9-10-11-12-13-14-15-16-20-29-24(27)26(6-2,7-3)25(28)30-2
InchiKey: HXRLQDURAGKEHQ-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-194.18	kJ/mol	Joback Method
hf	-853.26	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.171		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	975.29	K	Joback Method
tc	1194.04	K	Joback Method
tf	568.46	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.60	J/mol×K	975.29	Joback Method
cpg	1261.12	J/mol×K	1011.75	Joback Method
cpg	1277.24	J/mol×K	1048.21	Joback Method
cpg	1292.02	J/mol×K	1084.66	Joback Method
cpg	1305.54	J/mol×K	1121.12	Joback Method
cpg	1317.86	J/mol×K	1157.58	Joback Method
cpg	1329.05	J/mol×K	1194.04	Joback Method
dvisc	0.0002647	Pa×s	568.46	Joback Method

dvisc	0.0001319	Pa×s	636.26	Joback Method
dvisc	0.0000751	Pa×s	704.07	Joback Method
dvisc	0.0000472	Pa×s	771.88	Joback Method
dvisc	0.0000320	Pa×s	839.68	Joback Method
dvisc	0.0000230	Pa×s	907.49	Joback Method
dvisc	0.0000173	Pa×s	975.29	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=U370020&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