Diethylmalonic acid, hexadecyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C32H54O5/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-23-26-35-30(33)32(7-2,8
InchiKey: LWAJEPXWMBSOKJ-UHFFFAOYSA-N
Formula: C32H54O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 518.77

Physical Properties

Property code	Value	Unit	Source
gf	-251.10	kJ/mol	Joback Method
hf	-1114.60	kJ/mol	Joback Method
hfus	68.11	kJ/mol	Joback Method
hvap	108.80	kJ/mol	Joback Method
log10ws	-10.27		Crippen Method
logp	9.210		Crippen Method
mcvol	458.730	ml/mol	McGowan Method
pc	667.01	kPa	Joback Method
rinpol	3347.00		NIST Webbook
tb	1134.55	K	Joback Method
tc	1414.02	K	Joback Method
tf	643.31	K	Joback Method
vc	1.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.41	J/mol×K	1134.55	Joback Method
cpg	1720.95	J/mol×K	1367.44	Joback Method
cpg	1711.54	J/mol×K	1320.86	Joback Method
cpg	1700.14	J/mol×K	1274.28	Joback Method
cpg	1686.59	J/mol×K	1227.71	Joback Method
cpg	1670.73	J/mol×K	1181.13	Joback Method
cpg	1728.53	J/mol×K	1414.02	Joback Method
dvisc	0.0000043	Pa×s	1134.55	Joback Method
dvisc	0.0000058	Pa×s	1052.68	Joback Method

dvisc	0.0000083	Pa×s	970.80	Joback Method
dvisc	0.0000126	Pa×s	888.93	Joback Method
dvisc	0.0000210	Pa×s	807.06	Joback Method
dvisc	0.0000391	Pa×s	725.18	Joback Method
dvisc	0.0000852	Pa×s	643.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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