Dimethylmalonic acid, heptadecyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C31H52O5/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-34-29(32)31(4,5)
InchiKey: VGXOFRSHXRJYRL-UHFFFAOYSA-N
Formula: C31H52O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 504.74

Physical Properties

Property code	Value	Unit	Source
gf	-259.52	kJ/mol	Joback Method
hf	-1093.96	kJ/mol	Joback Method
hfus	65.52	kJ/mol	Joback Method
hvap	106.58	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.820		Crippen Method
mcvol	444.640	ml/mol	McGowan Method
pc	701.35	kPa	Joback Method
rinpol	3276.00		NIST Webbook
rinpol	3276.00		NIST Webbook
tb	1111.67	K	Joback Method
tc	1378.31	K	Joback Method
tf	632.04	K	Joback Method
vc	1.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1588.64	J/mol×K	1111.67	Joback Method
cpg	1606.61	J/mol×K	1156.11	Joback Method
cpg	1622.30	J/mol×K	1200.55	Joback Method
cpg	1635.87	J/mol×K	1244.99	Joback Method
cpg	1647.42	J/mol×K	1289.43	Joback Method
cpg	1657.10	J/mol×K	1333.87	Joback Method
cpg	1665.04	J/mol×K	1378.31	Joback Method
dvisc	0.0000986	Pa×s	632.04	Joback Method

dvisc	0.0000455	Pa×s	711.98	Joback Method
dvisc	0.0000246	Pa×s	791.92	Joback Method
dvisc	0.0000149	Pa×s	871.86	Joback Method
dvisc	0.0000098	Pa×s	951.79	Joback Method
dvisc	0.0000069	Pa×s	1031.73	Joback Method
dvisc	0.0000051	Pa×s	1111.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361865&Units=SI

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