Dimethylmalonic acid, 2-isopropoxyphenyl undecyl ester

Inchi: InChI=1S/C25H40O5/c1-6-7-8-9-10-11-12-13-16-19-28-23(26)25(4,5)24(27)30-22-18-15-

InchiKey: MIUVIGLLPBIWQT-UHFFFAOYSA-N

Formula: C25H40O5

SMILES: CCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 420.58

Physical Properties

Property code	Value	Unit	Source
gf	-310.04	kJ/mol	Joback Method
hf	-970.12	kJ/mol	Joback Method
hfus	49.98	kJ/mol	Joback Method
hvap	93.22	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.479		Crippen Method
mcvol	360.100	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2655.00		NIST Webbook
tb	974.39	K	Joback Method
tc	1193.14	K	Joback Method
tf	564.42	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.32	J/mol×K	974.39	Joback Method
cpg	1227.83	J/mol×K	1010.85	Joback Method
cpg	1242.82	J/mol×K	1047.31	Joback Method
cpg	1256.33	J/mol×K	1083.77	Joback Method
cpg	1268.43	J/mol×K	1120.22	Joback Method
cpg	1279.17	J/mol×K	1156.68	Joback Method
cpg	1288.59	J/mol×K	1193.14	Joback Method
dvisc	0.0002272	Pa×s	564.42	Joback Method
dvisc	0.0001101	Pa×s	632.75	Joback Method

dvisc	0.0000615	Pa×s	701.08	Joback Method
dvisc	0.0000381	Pa×s	769.40	Joback Method
dvisc	0.0000255	Pa×s	837.73	Joback Method
dvisc	0.0000181	Pa×s	906.06	Joback Method
dvisc	0.0000135	Pa×s	974.39	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=U361859&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