Dimethylmalonic acid, 2-isopropoxyphenyl tridecyl ester

Inchi: InChI=1S/C27H44O5/c1-6-7-8-9-10-11-12-13-14-15-18-21-30-25(28)27(4,5)26(29)32-24-
InchiKey: RPYOAPUFBGYSDH-UHFFFAOYSA-N
Formula: C27H44O5
SMILES: CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 448.64

Physical Properties

Property code	Value	Unit	Source
gf	-293.20	kJ/mol	Joback Method
hf	-1011.40	kJ/mol	Joback Method
hfus	55.16	kJ/mol	Joback Method
hvap	97.67	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.260		Crippen Method
mcvol	388.280	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	2851.00		NIST Webbook
rinpol	2851.00		NIST Webbook
tb	1020.15	K	Joback Method
tc	1249.96	K	Joback Method
tf	586.96	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1335.85	J/mol×K	1020.15	Joback Method
cpg	1352.72	J/mol×K	1058.45	Joback Method
cpg	1367.90	J/mol×K	1096.75	Joback Method
cpg	1381.44	J/mol×K	1135.06	Joback Method
cpg	1393.41	J/mol×K	1173.36	Joback Method
cpg	1403.88	J/mol×K	1211.66	Joback Method
cpg	1412.93	J/mol×K	1249.96	Joback Method
dvisc	0.0001734	Pa×s	586.96	Joback Method

dvisc	0.0000826	Pa×s	659.16	Joback Method
dvisc	0.0000456	Pa×s	731.36	Joback Method
dvisc	0.0000280	Pa×s	803.56	Joback Method
dvisc	0.0000186	Pa×s	875.75	Joback Method
dvisc	0.0000132	Pa×s	947.95	Joback Method
dvisc	0.0000098	Pa×s	1020.15	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=U361861&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