Dimethylmalonic acid, isobutyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C18H26O5/c1-12(2)11-21-16(19)18(5,6)17(20)23-15-10-8-7-9-14(15)22-13(3)4

InchiKey: ZQKUTJBHEGEGPX-UHFFFAOYSA-N

Formula: C18H26O5

SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-371.42	kJ/mol	Joback Method
hf	-830.92	kJ/mol	Joback Method
hfus	28.33	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.605		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	813.79	K	Joback Method
tc	1025.19	K	Joback Method
tf	470.53	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.45	J/mol×K	813.79	Joback Method
cpg	808.27	J/mol×K	849.02	Joback Method
cpg	822.86	J/mol×K	884.26	Joback Method
cpg	836.25	J/mol×K	919.49	Joback Method
cpg	848.47	J/mol×K	954.72	Joback Method
cpg	859.53	J/mol×K	989.96	Joback Method
cpg	869.47	J/mol×K	1025.19	Joback Method
dvisc	0.0006239	Pa×s	470.53	Joback Method

dvisc	0.0003011	Pa×s	527.74	Joback Method
dvisc	0.0001676	Pa×s	584.95	Joback Method
dvisc	0.0001035	Pa×s	642.16	Joback Method
dvisc	0.0000692	Pa×s	699.37	Joback Method
dvisc	0.0000492	Pa×s	756.58	Joback Method
dvisc	0.0000366	Pa×s	813.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361851&Units=SI
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

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