Dimethylmalonic acid, di(2-isopropoxyphenyl) ester

Inchi: InChI=1S/C23H28O6/c1-15(2)26-17-11-7-9-13-19(17)28-21(24)23(5,6)22(25)29-20-14-1
InchiKey: FHGYBXUZRQNWCC-UHFFFAOYSA-N
Formula: C23H28O6
SMILES: CC(C)Oc1ccccc1OC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 400.46

Physical Properties

Property code	Value	Unit	Source
gf	-331.54	kJ/mol	Joback Method
hf	-841.28	kJ/mol	Joback Method
hfus	36.12	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.798		Crippen Method
mcvol	314.030	ml/mol	McGowan Method
pc	1370.73	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	982.27	K	Joback Method
tc	1215.28	K	Joback Method
tf	588.05	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.38	J/mol×K	982.27	Joback Method
cpg	1024.04	J/mol×K	1021.10	Joback Method
cpg	1035.03	J/mol×K	1059.94	Joback Method
cpg	1044.38	J/mol×K	1098.77	Joback Method
cpg	1052.12	J/mol×K	1137.61	Joback Method
cpg	1058.30	J/mol×K	1176.44	Joback Method
cpg	1062.94	J/mol×K	1215.28	Joback Method
dvisc	0.0001668	Pa×s	588.05	Joback Method
dvisc	0.0000881	Pa×s	653.75	Joback Method

dvisc	0.0000522	Pa×s	719.46	Joback Method
dvisc	0.0000338	Pa×s	785.16	Joback Method
dvisc	0.0000234	Pa×s	850.86	Joback Method
dvisc	0.0000171	Pa×s	916.57	Joback Method
dvisc	0.0000130	Pa×s	982.27	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=U361866&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