Dimethylmalonic acid, 2-isopropoxyphenyl propyl ester

Inchi: InChI=1S/C17H24O5/c1-6-11-20-15(18)17(4,5)16(19)22-14-10-8-7-9-13(14)21-12(2)3/h7
InchiKey: YQLZNIGRZGYMNG-UHFFFAOYSA-N
Formula: C17H24O5
SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 308.37

Physical Properties

Property code	Value	Unit	Source
gf	-377.40	kJ/mol	Joback Method
hf	-805.00	kJ/mol	Joback Method
hfus	29.26	kJ/mol	Joback Method
hvap	75.41	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.359		Crippen Method
mcvol	247.380	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook
tb	791.35	K	Joback Method
tc	1001.53	K	Joback Method
tf	474.26	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.88	J/mol×K	791.35	Joback Method
cpg	750.34	J/mol×K	826.38	Joback Method
cpg	764.65	J/mol×K	861.41	Joback Method
cpg	777.82	J/mol×K	896.44	Joback Method
cpg	789.89	J/mol×K	931.47	Joback Method
cpg	800.86	J/mol×K	966.50	Joback Method
cpg	810.76	J/mol×K	1001.53	Joback Method
dvisc	0.0005979	Pa×s	474.26	Joback Method

dvisc	0.0003151	Pa×s	527.11	Joback Method
dvisc	0.0001866	Pa×s	579.96	Joback Method
dvisc	0.0001206	Pa×s	632.80	Joback Method
dvisc	0.0000834	Pa×s	685.65	Joback Method
dvisc	0.0000608	Pa×s	738.50	Joback Method
dvisc	0.0000462	Pa×s	791.35	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=U361850&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