Dimethylmalonic acid, isohexyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C20H30O5/c1-14(2)10-9-13-23-18(21)20(5,6)19(22)25-17-12-8-7-11-16(17)24-

InchiKey: HRCWFXDHZHLTDF-UHFFFAOYSA-N

Formula: C20H30O5

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

Mol. weight [g/mol]: 350.45

Physical Properties

Property code	Value	Unit	Source
gf	-354.58	kJ/mol	Joback Method
hf	-872.20	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	81.70	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.385		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	859.55	K	Joback Method
tc	1069.31	K	Joback Method
tf	493.07	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.98	J/mol×K	859.55	Joback Method
cpg	976.52	J/mol×K	1034.35	Joback Method
cpg	965.46	J/mol×K	999.39	Joback Method
cpg	953.21	J/mol×K	964.43	Joback Method
cpg	939.73	J/mol×K	929.47	Joback Method
cpg	925.00	J/mol×K	894.51	Joback Method
cpg	986.41	J/mol×K	1069.31	Joback Method
dvisc	0.0000271	Pa×s	859.55	Joback Method

dvisc	0.0000365	Pa×s	798.47	Joback Method
dvisc	0.0000517	Pa×s	737.39	Joback Method
dvisc	0.0000779	Pa×s	676.31	Joback Method
dvisc	0.0001273	Pa×s	615.23	Joback Method
dvisc	0.0002321	Pa×s	554.15	Joback Method
dvisc	0.0004909	Pa×s	493.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361854&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