Dimethylmalonic acid, 2-isopropoxyphenyl pentyl ester

Inchi: InChI=1S/C19H28O5/c1-6-7-10-13-22-17(20)19(4,5)18(21)24-16-12-9-8-11-15(16)23-14
InchiKey: GDZGYXNMSXIHKC-UHFFFAOYSA-N
Formula: C19H28O5
SMILES: CCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-360.56	kJ/mol	Joback Method
hf	-846.28	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.139		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2081.00		NIST Webbook
tb	837.11	K	Joback Method
tc	1045.01	K	Joback Method
tf	496.80	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.79	J/mol×K	837.11	Joback Method
cpg	916.72	J/mol×K	1010.36	Joback Method
cpg	905.66	J/mol×K	975.71	Joback Method
cpg	893.46	J/mol×K	941.06	Joback Method
cpg	880.10	J/mol×K	906.41	Joback Method
cpg	865.56	J/mol×K	871.76	Joback Method
cpg	926.68	J/mol×K	1045.01	Joback Method
dvisc	0.0000344	Pa×s	837.11	Joback Method
dvisc	0.0000455	Pa×s	780.39	Joback Method

dvisc	0.0000628	Pa×s	723.67	Joback Method
dvisc	0.0000917	Pa×s	666.96	Joback Method
dvisc	0.0001436	Pa×s	610.24	Joback Method
dvisc	0.0002466	Pa×s	553.52	Joback Method
dvisc	0.0004790	Pa×s	496.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361853&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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