Dimethylmalonic acid, 2-isopropoxyphenyl nonyl ester

Inchi: InChI=1S/C23H36O5/c1-6-7-8-9-10-11-14-17-26-21(24)23(4,5)22(25)28-20-16-13-12-15-
InchiKey: INSZAOMTRODRNO-UHFFFAOYSA-N
Formula: C23H36O5
SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-326.88	kJ/mol	Joback Method
hf	-928.84	kJ/mol	Joback Method
hfus	44.80	kJ/mol	Joback Method
hvap	88.77	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.699		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2461.00		NIST Webbook
tb	928.63	K	Joback Method
tc	1140.38	K	Joback Method
tf	541.88	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.52	J/mol×K	928.63	Joback Method
cpg	1104.74	J/mol×K	963.92	Joback Method
cpg	1119.58	J/mol×K	999.21	Joback Method
cpg	1133.07	J/mol×K	1034.51	Joback Method
cpg	1145.26	J/mol×K	1069.80	Joback Method
cpg	1156.18	J/mol×K	1105.09	Joback Method
cpg	1165.87	J/mol×K	1140.38	Joback Method
dvisc	0.0002947	Pa×s	541.88	Joback Method
dvisc	0.0001456	Pa×s	606.34	Joback Method

dvisc	0.0000823	Pa×s	670.80	Joback Method
dvisc	0.0000515	Pa×s	735.25	Joback Method
dvisc	0.0000347	Pa×s	799.71	Joback Method
dvisc	0.0000248	Pa×s	864.17	Joback Method
dvisc	0.0000186	Pa×s	928.63	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=U361857&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

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