

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/molxK	928.63	Joback Method
cpg	1104.74	J/molxK	963.92	Joback Method
cpg	1119.58	J/molxK	999.21	Joback Method
cpg	1133.07	J/molxK	1034.51	Joback Method
cpg	1145.26	J/molxK	1069.80	Joback Method
cpg	1156.18	J/molxK	1105.09	Joback Method
cpg	1165.87	J/molxK	1140.38	Joback Method
dvisc	0.0002947	Paxs	541.88	Joback Method
dvisc	0.0001456	Paxs	606.34	Joback Method

dvisc	0.0000823	Paxs	670.80	Joback Method
dvisc	0.0000515	Paxs	735.25	Joback Method
dvisc	0.0000347	Paxs	799.71	Joback Method
dvisc	0.0000248	Paxs	864.17	Joback Method
dvisc	0.0000186	Paxs	928.63	Joback Method

Sources

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/ci9903071
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

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