Dimethylmalonic acid, 2-isopropoxyphenyl octyl ester

Inchi: InChI=1S/C22H34O5/c1-6-7-8-9-10-13-16-25-20(23)22(4,5)21(24)27-19-15-12-11-14-18

InchiKey: CBKVLWADKPGLEQ-UHFFFAOYSA-N

Formula: C22H34O5

SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-335.30	kJ/mol	Joback Method
hf	-908.20	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	86.54	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.309		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	2362.00		NIST Webbook
tb	905.75	K	Joback Method
tc	1115.36	K	Joback Method
tf	530.61	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.89	J/mol×K	905.75	Joback Method
cpg	1044.00	J/mol×K	940.68	Joback Method
cpg	1058.77	J/mol×K	975.62	Joback Method
cpg	1072.24	J/mol×K	1010.55	Joback Method
cpg	1084.46	J/mol×K	1045.49	Joback Method
cpg	1095.44	J/mol×K	1080.42	Joback Method
cpg	1105.24	J/mol×K	1115.36	Joback Method
dvisc	0.0003343	Pa×s	530.61	Joback Method
dvisc	0.0001668	Pa×s	593.13	Joback Method

dvisc	0.0000950	Pa×s	655.66	Joback Method
dvisc	0.0000597	Pa×s	718.18	Joback Method
dvisc	0.0000404	Pa×s	780.70	Joback Method
dvisc	0.0000290	Pa×s	843.23	Joback Method
dvisc	0.0000217	Pa×s	905.75	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=U361856&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