Diethylmalonic acid, di(2-isopropoxyphenyl) ester

Inchi: InChI=1S/C25H32O6/c1-7-25(8-2,23(26)30-21-15-11-9-13-19(21)28-17(3)4)24(27)31-22-
InchiKey: LRFCRCDFEBRGMX-UHFFFAOYSA-N
Formula: C25H32O6
SMILES: CCC(CC)(C(=O)Oc1ccccc1OC(C)C)C(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]: 428.52

Physical Properties

Property code	Value	Unit	Source
gf	-314.70	kJ/mol	Joback Method
hf	-882.56	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	98.18	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.578		Crippen Method
mcvol	342.210	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	1028.03	K	Joback Method
tc	1263.21	K	Joback Method
tf	610.59	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.50	J/mol×K	1028.03	Joback Method
cpg	1142.87	J/mol×K	1067.23	Joback Method
cpg	1153.48	J/mol×K	1106.42	Joback Method
cpg	1162.36	J/mol×K	1145.62	Joback Method
cpg	1169.58	J/mol×K	1184.82	Joback Method
cpg	1175.16	J/mol×K	1224.01	Joback Method
cpg	1179.15	J/mol×K	1263.21	Joback Method
dvisc	0.0001290	Pa×s	610.59	Joback Method

dvisc	0.0000669	Pa×s	680.16	Joback Method
dvisc	0.0000391	Pa×s	749.74	Joback Method
dvisc	0.0000251	Pa×s	819.31	Joback Method
dvisc	0.0000172	Pa×s	888.88	Joback Method
dvisc	0.0000125	Pa×s	958.46	Joback Method
dvisc	0.0000095	Pa×s	1028.03	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=U369596&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