Isophthalic acid, di(2-isopropoxyphenyl) ester

Inchi: InChI=1S/C26H26O6/c1-17(2)29-21-12-5-7-14-23(21)31-25(27)19-10-9-11-20(16-19)26(
InchiKey: MJPAAZKXNHVXHG-UHFFFAOYSA-N
Formula: C26H26O6
SMILES: CC(C)Oc1ccccc1OC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]: 434.48

Physical Properties

Property code	Value	Unit	Source
gf	-206.34	kJ/mol	Joback Method
hf	-669.39	kJ/mol	Joback Method
hfus	44.96	kJ/mol	Joback Method
hvap	104.64	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	5.699		Crippen Method
mcvol	332.540	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	3293.00		NIST Webbook
tb	1085.80	K	Joback Method
tc	1336.43	K	Joback Method
tf	658.38	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.94	J/mol×K	1085.80	Joback Method
cpg	1081.29	J/mol×K	1127.57	Joback Method
cpg	1087.54	J/mol×K	1169.34	Joback Method
cpg	1091.74	J/mol×K	1211.11	Joback Method
cpg	1093.90	J/mol×K	1252.89	Joback Method
cpg	1094.04	J/mol×K	1294.66	Joback Method
cpg	1092.21	J/mol×K	1336.43	Joback Method
dvisc	0.0001103	Pa×s	658.38	Joback Method
dvisc	0.0000631	Pa×s	729.62	Joback Method

dvisc	0.0000399	Pa×s	800.85	Joback Method
dvisc	0.0000272	Pa×s	872.09	Joback Method
dvisc	0.0000196	Pa×s	943.33	Joback Method
dvisc	0.0000148	Pa×s	1014.56	Joback Method
dvisc	0.0000116	Pa×s	1085.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344437&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

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