Isophthalic acid, di(2-isopropylphenyl) ester

Inchi: InChI=1S/C26H26O4/c1-17(2)21-12-5-7-14-23(21)29-25(27)19-10-9-11-20(16-19)26(28)
InchiKey: JNEANCAZOPNWOB-UHFFFAOYSA-N
Formula: C26H26O4
SMILES: CC(C)c1ccccc1OC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1
Mol. weight [g/mol]: 402.48

Physical Properties

Property code	Value	Unit	Source
gf	3.66	kJ/mol	Joback Method
hf	-404.95	kJ/mol	Joback Method
hfus	42.58	kJ/mol	Joback Method
hvap	99.82	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.372		Crippen Method
mcvol	320.800	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	3127.00		NIST Webbook
rinpol	3127.00		NIST Webbook
tb	1040.96	K	Joback Method
tc	1290.06	K	Joback Method
tf	613.92	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.26	J/mol×K	1040.96	Joback Method
cpg	1036.89	J/mol×K	1082.48	Joback Method
cpg	1046.89	J/mol×K	1123.99	Joback Method
cpg	1055.33	J/mol×K	1165.51	Joback Method
cpg	1062.29	J/mol×K	1207.03	Joback Method
cpg	1067.83	J/mol×K	1248.55	Joback Method
cpg	1072.03	J/mol×K	1290.06	Joback Method
dvisc	0.0002246	Pa×s	613.92	Joback Method

dvisc	0.0001239	Pa×s	685.09	Joback Method
dvisc	0.0000764	Pa×s	756.27	Joback Method
dvisc	0.0000512	Pa×s	827.44	Joback Method
dvisc	0.0000366	Pa×s	898.61	Joback Method
dvisc	0.0000274	Pa×s	969.79	Joback Method
dvisc	0.0000214	Pa×s	1040.96	Joback Method

Sources

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=U344642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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