1,2-Cyclohexanedicarboxylic acid, di(2-isopropylphenyl) ester

Inchi: InChI=1S/C26H32O4/c1-17(2)19-11-7-9-15-23(19)29-25(27)21-13-5-6-14-22(21)26(28)3

InchiKey: DMFXNIFYFQLTMA-UHFFFAOYSA-N

Formula: C26H32O4

SMILES: CC(C)c1ccccc1OC(=O)C1CCCCC1C(=O)Oc1ccccc1C(C)C

Mol. weight [g/mol]: 408.53

Physical Properties

Property code	Value	Unit	Source
gf	-82.38	kJ/mol	Joback Method
hf	-596.03	kJ/mol	Joback Method
hfus	41.83	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	6.251		Crippen Method
mcvol	333.700	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	1024.18	K	Joback Method
tc	1268.34	K	Joback Method
tf	578.12	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.60	J/mol×K	1024.18	Joback Method
cpg	1148.43	J/mol×K	1064.87	Joback Method
cpg	1160.25	J/mol×K	1105.57	Joback Method
cpg	1170.13	J/mol×K	1146.26	Joback Method
cpg	1178.13	J/mol×K	1186.96	Joback Method
cpg	1184.30	J/mol×K	1227.65	Joback Method
cpg	1188.72	J/mol×K	1268.34	Joback Method
dvisc	0.0003634	Pa×s	578.12	Joback Method

dvisc	0.0001855	Pa×s	652.46	Joback Method
dvisc	0.0001087	Pa×s	726.81	Joback Method
dvisc	0.0000703	Pa×s	801.15	Joback Method
dvisc	0.0000490	Pa×s	875.49	Joback Method
dvisc	0.0000361	Pa×s	949.84	Joback Method
dvisc	0.0000278	Pa×s	1024.18	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=U339707&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