

1,2-Cyclohexanedicarboxylic acid, di(4-isopropoxyphenyl) diester

Other names:	1,2-Cyclohexanedicarboxylic acid, di(4-isopropylphenyl) ester
Inchi:	InChI=1S/C26H32O6/c1-17(2)29-19-9-13-21(14-10-19)31-25(27)23-7-5-6-8-24(23)26(28)
InchiKey:	IAPBHLNVYJWTHP-UHFFFAOYSA-N
Formula:	C26H32O6
SMILES:	CC(C)Oc1ccc(OC(=O)C2CCCCC2C(=O)Oc2ccc(OC(C)C)cc2)cc1
Mol. weight [g/mol]:	440.53

Physical Properties

Property code	Value	Unit	Source
gf	-292.38	kJ/mol	Joback Method
hf	-860.47	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	101.82	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.578		Crippen Method
mcvol	345.440	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	3038.00		NIST Webbook
tb	1069.02	K	Joback Method
tc	1315.15	K	Joback Method
tf	622.58	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1185.41	J/molxK	1069.02	Joback Method
cpg	1195.76	J/molxK	1110.04	Joback Method
cpg	1203.66	J/molxK	1151.06	Joback Method
cpg	1209.13	J/molxK	1192.09	Joback Method
cpg	1212.19	J/molxK	1233.11	Joback Method
cpg	1212.85	J/molxK	1274.13	Joback Method
cpg	1211.13	J/molxK	1315.15	Joback Method
dvisc	0.0001759	Paxs	622.58	Joback Method

dvisc	0.0000940	Paxs	696.99	Joback Method
dvisc	0.0000566	Paxs	771.39	Joback Method
dvisc	0.0000373	Paxs	845.80	Joback Method
dvisc	0.0000263	Paxs	920.21	Joback Method
dvisc	0.0000196	Paxs	994.61	Joback Method
dvisc	0.0000151	Paxs	1069.02	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=U339582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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