

1,2-Cyclohexanedicarboxylic acid, di(4-methoxyphenyl) ester

Inchi: InChI=1S/C22H24O6/c1-25-15-7-11-17(12-8-15)27-21(23)19-5-3-4-6-20(19)22(24)28-18
InchiKey: OLTMPDUMUWOPJJ-UHFFFAOYSA-N
Formula: C22H24O6
SMILES: COc1ccc(OC(=O)C2CCCCC2C(=O)Oc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 384.42

Physical Properties

Property code	Value	Unit	Source
gf	-321.18	kJ/mol	Joback Method
hf	-767.35	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	93.69	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.021		Crippen Method
mcvol	289.080	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	3185.00		NIST Webbook
rinpol	3185.00		NIST Webbook
tb	978.38	K	Joback Method
tc	1220.75	K	Joback Method
tf	607.50	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.16	J/molxK	978.38	Joback Method
cpg	960.38	J/molxK	1018.78	Joback Method
cpg	970.45	J/molxK	1059.17	Joback Method
cpg	978.37	J/molxK	1099.57	Joback Method
cpg	984.14	J/molxK	1139.96	Joback Method
cpg	987.76	J/molxK	1180.36	Joback Method
cpg	989.22	J/molxK	1220.75	Joback Method
dvisc	0.0002444	Paxs	607.50	Joback Method

dvisc	0.0001502	Paxs	669.31	Joback Method
dvisc	0.0001002	Paxs	731.13	Joback Method
dvisc	0.0000712	Paxs	792.94	Joback Method
dvisc	0.0000532	Paxs	854.75	Joback Method
dvisc	0.0000413	Paxs	916.57	Joback Method
dvisc	0.0000331	Paxs	978.38	Joback Method

Sources

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=U339677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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