1,2-Cyclohexanedicarboxylic acid, 2,6-dimethoxyphenyl isobutyl ester

Inchi: InChI=1S/C20H28O6/c1-13(2)12-25-19(21)14-8-5-6-9-15(14)20(22)26-18-16(23-3)10-7-1

InchiKey: PIRZCCPJHXBJOA-UHFFFAOYSA-N

Formula: C20H28O6

SMILES: COc1cccc(OC)c1OC(=O)C1CCCCC1C(=O)OCC(C)C

Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-452.87	kJ/mol	Joback Method
hf	-967.88	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.615		Crippen Method
mcvol	284.660	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	905.50	K	Joback Method
tc	1127.06	K	Joback Method
tf	543.54	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.71	J/mol×K	905.50	Joback Method
cpg	994.17	J/mol×K	1090.13	Joback Method
cpg	985.95	J/mol×K	1053.20	Joback Method
cpg	975.88	J/mol×K	1016.28	Joback Method
cpg	963.97	J/mol×K	979.35	Joback Method
cpg	950.24	J/mol×K	942.43	Joback Method
cpg	1000.53	J/mol×K	1127.06	Joback Method
dvisc	0.0000387	Pa×s	905.50	Joback Method

dvisc	0.0000490	Pa×s	845.17	Joback Method
dvisc	0.0000645	Pa×s	784.85	Joback Method
dvisc	0.0000889	Pa×s	724.52	Joback Method
dvisc	0.0001298	Pa×s	664.19	Joback Method
dvisc	0.0002045	Pa×s	603.87	Joback Method
dvisc	0.0003562	Pa×s	543.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339931&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