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

Inchi: InChI=1S/C21H30O6/c1-4-5-8-14-26-20(22)15-10-6-7-11-16(15)21(23)27-19-17(24-2)12

InchiKey: BTHDSOSWIREZMB-UHFFFAOYSA-N

Formula: C21H30O6

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
gf	-442.01	kJ/mol	Joback Method
hf	-983.24	kJ/mol	Joback Method
hfus	44.26	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.149		Crippen Method
mcvol	298.750	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	928.82	K	Joback Method
tc	1148.40	K	Joback Method
tf	569.81	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.00	J/mol×K	928.82	Joback Method
cpg	1009.21	J/mol×K	965.42	Joback Method
cpg	1022.59	J/mol×K	1002.01	Joback Method
cpg	1034.14	J/mol×K	1038.61	Joback Method
cpg	1043.85	J/mol×K	1075.21	Joback Method
cpg	1051.69	J/mol×K	1111.80	Joback Method
cpg	1057.67	J/mol×K	1148.40	Joback Method
dvisc	0.0002962	Pa×s	569.81	Joback Method

dvisc	0.0001773	Pa×s	629.64	Joback Method
dvisc	0.0001160	Pa×s	689.48	Joback Method
dvisc	0.0000813	Pa×s	749.31	Joback Method
dvisc	0.0000600	Pa×s	809.15	Joback Method
dvisc	0.0000462	Pa×s	868.98	Joback Method
dvisc	0.0000368	Pa×s	928.82	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=U339933&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