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

Inchi: InChI=1S/C24H36O6/c1-4-5-6-7-8-11-17-29-23(25)18-13-9-10-14-19(18)24(26)30-22-20

InchiKey: JGABBUKGJHSTSK-UHFFFAOYSA-N

Formula: C24H36O6

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

Mol. weight [g/mol]: 420.54

Physical Properties

Property code	Value	Unit	Source
gf	-416.75	kJ/mol	Joback Method
hf	-1045.16	kJ/mol	Joback Method
hfus	52.03	kJ/mol	Joback Method
hvap	95.87	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.319		Crippen Method
mcvol	341.020	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	997.46	K	Joback Method
tc	1222.78	K	Joback Method
tf	603.62	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1175.63	J/mol×K	997.46	Joback Method
cpg	1227.03	J/mol×K	1185.23	Joback Method
cpg	1220.94	J/mol×K	1147.67	Joback Method
cpg	1212.75	J/mol×K	1110.12	Joback Method
cpg	1202.47	J/mol×K	1072.57	Joback Method
cpg	1190.10	J/mol×K	1035.01	Joback Method
cpg	1231.02	J/mol×K	1222.78	Joback Method
dvisc	0.0000238	Pa×s	997.46	Joback Method

dvisc	0.0000301	Pa×s	931.82	Joback Method
dvisc	0.0000396	Pa×s	866.18	Joback Method
dvisc	0.0000544	Pa×s	800.54	Joback Method
dvisc	0.0000791	Pa×s	734.90	Joback Method
dvisc	0.0001239	Pa×s	669.26	Joback Method
dvisc	0.0002138	Pa×s	603.62	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=U339936&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