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

Inchi: InChI=1S/C19H26O6/c1-4-12-24-18(20)13-8-5-6-9-14(13)19(21)25-17-15(22-2)10-7-11-1

InchiKey: FDBADGFNRJVGGQ-UHFFFAOYSA-N

Formula: C19H26O6

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

Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-458.85	kJ/mol	Joback Method
hf	-941.96	kJ/mol	Joback Method
hfus	39.08	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.369		Crippen Method
mcvol	270.570	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2518.00		NIST Webbook
tb	883.06	K	Joback Method
tc	1103.00	K	Joback Method
tf	547.27	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.93	J/mol×K	883.06	Joback Method
cpg	935.74	J/mol×K	1066.34	Joback Method
cpg	927.05	J/mol×K	1029.68	Joback Method
cpg	916.60	J/mol×K	993.03	Joback Method
cpg	904.42	J/mol×K	956.37	Joback Method
cpg	890.53	J/mol×K	919.72	Joback Method
cpg	942.65	J/mol×K	1103.00	Joback Method
dvisc	0.0000486	Pa×s	883.06	Joback Method
dvisc	0.0000606	Pa×s	827.10	Joback Method

dvisc	0.0000781	Pa×s	771.13	Joback Method
dvisc	0.0001047	Pa×s	715.16	Joback Method
dvisc	0.0001476	Pa×s	659.20	Joback Method
dvisc	0.0002215	Pa×s	603.24	Joback Method
dvisc	0.0003615	Pa×s	547.27	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=U339930&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