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

Inchi: InChI=1S/C22H32O6/c1-4-5-6-9-15-27-21(23)16-11-7-8-12-17(16)22(24)28-20-18(25-2)1

InchiKey: FVTIQQVLQUWOJI-UHFFFAOYSA-N

Formula: C22H32O6

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

Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-433.59	kJ/mol	Joback Method
hf	-1003.88	kJ/mol	Joback Method
hfus	46.85	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.539		Crippen Method
mcvol	312.840	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	951.70	K	Joback Method
tc	1172.30	K	Joback Method
tf	581.08	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.21	J/mol×K	951.70	Joback Method
cpg	1069.19	J/mol×K	988.47	Joback Method
cpg	1082.27	J/mol×K	1025.23	Joback Method
cpg	1093.44	J/mol×K	1062.00	Joback Method
cpg	1102.70	J/mol×K	1098.77	Joback Method
cpg	1110.03	J/mol×K	1135.53	Joback Method
cpg	1115.43	J/mol×K	1172.30	Joback Method
dvisc	0.0002666	Pa×s	581.08	Joback Method

dvisc	0.0001578	Pa×s	642.85	Joback Method
dvisc	0.0001024	Pa×s	704.62	Joback Method
dvisc	0.0000713	Pa×s	766.39	Joback Method
dvisc	0.0000524	Pa×s	828.16	Joback Method
dvisc	0.0000401	Pa×s	889.93	Joback Method
dvisc	0.0000319	Pa×s	951.70	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=U339934&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