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

Inchi: InChI=1S/C23H34O6/c1-4-5-6-7-10-16-28-22(24)17-12-8-9-13-18(17)23(25)29-21-19(26
InchiKey: NSZWUWWAYVQEPQ-UHFFFAOYSA-N
Formula: C23H34O6
SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 406.51

Physical Properties

Property code	Value	Unit	Source
gf	-425.17	kJ/mol	Joback Method
hf	-1024.52	kJ/mol	Joback Method
hfus	49.44	kJ/mol	Joback Method
hvap	93.64	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.929		Crippen Method
mcvol	326.930	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2888.00		NIST Webbook
tb	974.58	K	Joback Method
tc	1197.08	K	Joback Method
tf	592.35	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.78	J/mol×K	974.58	Joback Method
cpg	1129.50	J/mol×K	1011.66	Joback Method
cpg	1142.25	J/mol×K	1048.75	Joback Method
cpg	1153.00	J/mol×K	1085.83	Joback Method
cpg	1161.75	J/mol×K	1122.91	Joback Method
cpg	1168.50	J/mol×K	1159.99	Joback Method
cpg	1173.24	J/mol×K	1197.08	Joback Method
dvisc	0.0002391	Pa×s	592.35	Joback Method
dvisc	0.0001400	Pa×s	656.05	Joback Method

dvisc	0.0000901	Pa×s	719.76	Joback Method
dvisc	0.0000623	Pa×s	783.46	Joback Method
dvisc	0.0000456	Pa×s	847.17	Joback Method
dvisc	0.0000348	Pa×s	910.88	Joback Method
dvisc	0.0000275	Pa×s	974.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339935&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