Isophthalic acid, 2,6-dimethoxyphenyl isohexyl ester

Inchi: InChI=1S/C22H26O6/c1-15(2)8-7-13-27-21(23)16-9-5-10-17(14-16)22(24)28-20-18(25-3

InchiKey: KTNBULUUCNCXLA-UHFFFAOYSA-N

Formula: C22H26O6

SMILES: COc1cccc(OC)c1OC(=O)c1cccc(C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 386.44

Physical Properties

Property code	Value	Unit	Source
gf	-349.99	kJ/mol	Joback Method
hf	-818.08	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	93.85	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.516		Crippen Method
mcvol	299.940	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	3010.00		NIST Webbook
rinpol	3010.00		NIST Webbook
tb	968.04	K	Joback Method
tc	1194.73	K	Joback Method
tf	601.88	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	950.23	J/mol×K	968.04	Joback Method
cpg	994.82	J/mol×K	1156.94	Joback Method
cpg	989.28	J/mol×K	1119.16	Joback Method
cpg	982.05	J/mol×K	1081.38	Joback Method
cpg	973.12	J/mol×K	1043.60	Joback Method
cpg	962.52	J/mol×K	1005.82	Joback Method
cpg	998.67	J/mol×K	1194.73	Joback Method
dvisc	0.0000224	Pa×s	968.04	Joback Method

dvisc	0.0000282	Pa×s	907.01	Joback Method
dvisc	0.0000367	Pa×s	845.99	Joback Method
dvisc	0.0000498	Pa×s	784.96	Joback Method
dvisc	0.0000711	Pa×s	723.93	Joback Method
dvisc	0.0001083	Pa×s	662.91	Joback Method
dvisc	0.0001798	Pa×s	601.88	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=U344535&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