Isophthalic acid, 2,6-dimethoxyphenyl pentyl ester

Inchi: InChI=1S/C21H24O6/c1-4-5-6-13-26-20(22)15-9-7-10-16(14-15)21(23)27-19-17(24-2)11

InchiKey: ZPQCBSMKYCKPLM-UHFFFAOYSA-N

Formula: C21H24O6

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2c(OC)cccc2OC)c1

Mol. weight [g/mol]: 372.41

Physical Properties

Property code	Value	Unit	Source
gf	-355.97	kJ/mol	Joback Method
hf	-792.16	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	92.01	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.270		Crippen Method
mcvol	285.850	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2952.00		NIST Webbook
rinpol	2952.00		NIST Webbook
tb	945.60	K	Joback Method
tc	1169.94	K	Joback Method
tf	605.61	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.16	J/mol×K	945.60	Joback Method
cpg	903.51	J/mol×K	982.99	Joback Method
cpg	914.28	J/mol×K	1020.38	Joback Method
cpg	923.46	J/mol×K	1057.77	Joback Method
cpg	931.06	J/mol×K	1095.16	Joback Method
cpg	937.05	J/mol×K	1132.55	Joback Method
cpg	941.44	J/mol×K	1169.94	Joback Method
dvisc	0.0001879	Pa×s	605.61	Joback Method

dvisc	0.0001199	Pa×s	662.28	Joback Method
dvisc	0.0000821	Pa×s	718.94	Joback Method
dvisc	0.0000594	Pa×s	775.61	Joback Method
dvisc	0.0000449	Pa×s	832.27	Joback Method
dvisc	0.0000352	Pa×s	888.93	Joback Method
dvisc	0.0000284	Pa×s	945.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344534&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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