Isophthalic acid, 2-isopropoxyphenyl pentyl ester

Inchi: InChI=1S/C22H26O5/c1-4-5-8-14-25-21(23)17-10-9-11-18(15-17)22(24)27-20-13-7-6-12

InchiKey: PLIMPCQANUOFNE-UHFFFAOYSA-N

Formula: C22H26O5

SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1

Mol. weight [g/mol]: 370.44

Physical Properties

Property code	Value	Unit	Source
gf	-235.36	kJ/mol	Joback Method
hf	-674.39	kJ/mol	Joback Method
hfus	43.28	kJ/mol	Joback Method
hvap	90.78	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.040		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	940.64	K	Joback Method
tc	1165.59	K	Joback Method
tf	567.13	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.67	J/mol×K	940.64	Joback Method
cpg	977.19	J/mol×K	1128.10	Joback Method
cpg	969.59	J/mol×K	1090.61	Joback Method
cpg	960.56	J/mol×K	1053.12	Joback Method
cpg	950.08	J/mol×K	1015.62	Joback Method
cpg	938.12	J/mol×K	978.13	Joback Method
cpg	983.38	J/mol×K	1165.59	Joback Method
dvisc	0.0000295	Pa×s	940.64	Joback Method

dvisc	0.0000376	Pa×s	878.39	Joback Method
dvisc	0.0000499	Pa×s	816.14	Joback Method
dvisc	0.0000692	Pa×s	753.88	Joback Method
dvisc	0.0001020	Pa×s	691.63	Joback Method
dvisc	0.0001621	Pa×s	629.38	Joback Method
dvisc	0.0002854	Pa×s	567.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344429&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