Isophthalic acid, isohexyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C23H28O5/c1-16(2)9-8-14-26-22(24)18-10-7-11-19(15-18)23(25)28-21-13-6-5

InchiKey: KFLONDAZBWJKAY-UHFFFAOYSA-N

Formula: C23H28O5

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1

Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-229.38	kJ/mol	Joback Method
hf	-700.31	kJ/mol	Joback Method
hfus	42.35	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.286		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	963.08	K	Joback Method
tc	1190.21	K	Joback Method
tf	563.40	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.26	J/mol×K	963.08	Joback Method
cpg	997.72	J/mol×K	1000.94	Joback Method
cpg	1009.59	J/mol×K	1038.79	Joback Method
cpg	1019.92	J/mol×K	1076.65	Joback Method
cpg	1028.71	J/mol×K	1114.50	Joback Method
cpg	1036.01	J/mol×K	1152.36	Joback Method
cpg	1041.83	J/mol×K	1190.21	Joback Method
dvisc	0.0002788	Pa×s	563.40	Joback Method

dvisc	0.0001480	Pa×s	630.01	Joback Method
dvisc	0.0000887	Pa×s	696.63	Joback Method
dvisc	0.0000581	Pa×s	763.24	Joback Method
dvisc	0.0000407	Pa×s	829.85	Joback Method
dvisc	0.0000301	Pa×s	896.47	Joback Method
dvisc	0.0000232	Pa×s	963.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344430&Units=SI

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