Isophthalic acid, hexyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C23H28O5/c1-4-5-6-9-15-26-22(24)18-11-10-12-19(16-18)23(25)28-21-14-8-7

InchiKey: CVIDLRAMFVCQQE-UHFFFAOYSA-N

Formula: C23H28O5

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

Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-226.94	kJ/mol	Joback Method
hf	-695.03	kJ/mol	Joback Method
hfus	45.87	kJ/mol	Joback Method
hvap	93.00	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.430		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	963.52	K	Joback Method
tc	1188.96	K	Joback Method
tf	578.40	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.82	J/mol×K	963.52	Joback Method
cpg	997.23	J/mol×K	1001.09	Joback Method
cpg	1009.10	J/mol×K	1038.67	Joback Method
cpg	1019.45	J/mol×K	1076.24	Joback Method
cpg	1028.32	J/mol×K	1113.81	Joback Method
cpg	1035.71	J/mol×K	1151.39	Joback Method
cpg	1041.67	J/mol×K	1188.96	Joback Method
dvisc	0.0002556	Pa×s	578.40	Joback Method

dvisc	0.0001436	Pa×s	642.59	Joback Method
dvisc	0.0000896	Pa×s	706.77	Joback Method
dvisc	0.0000605	Pa×s	770.96	Joback Method
dvisc	0.0000434	Pa×s	835.15	Joback Method
dvisc	0.0000326	Pa×s	899.33	Joback Method
dvisc	0.0000255	Pa×s	963.52	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=U344431&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