Isophthalic acid, isobutyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C21H24O5/c1-14(2)13-24-20(22)16-8-7-9-17(12-16)21(23)26-19-11-6-5-10-18

InchiKey: XFSDQVDGYUQIHZ-UHFFFAOYSA-N

Formula: C21H24O5

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

Mol. weight [g/mol]: 356.41

Physical Properties

Property code	Value	Unit	Source
gf	-246.22	kJ/mol	Joback Method
hf	-659.03	kJ/mol	Joback Method
hfus	37.17	kJ/mol	Joback Method
hvap	88.16	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.506		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
tb	917.32	K	Joback Method
tc	1145.03	K	Joback Method
tf	540.86	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.56	J/mol×K	917.32	Joback Method
cpg	880.14	J/mol×K	955.27	Joback Method
cpg	892.22	J/mol×K	993.22	Joback Method
cpg	902.82	J/mol×K	1031.18	Joback Method
cpg	911.95	J/mol×K	1069.13	Joback Method
cpg	919.64	J/mol×K	1107.08	Joback Method
cpg	925.89	J/mol×K	1145.03	Joback Method
dvisc	0.0003486	Pa×s	540.86	Joback Method

dvisc	0.0001890	Pa×s	603.60	Joback Method
dvisc	0.0001150	Pa×s	666.35	Joback Method
dvisc	0.0000762	Pa×s	729.09	Joback Method
dvisc	0.0000539	Pa×s	791.83	Joback Method
dvisc	0.0000401	Pa×s	854.58	Joback Method
dvisc	0.0000311	Pa×s	917.32	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=U344427&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