Isophthalic acid, 2-isopropoxyphenyl octyl ester

Inchi: InChI=1S/C25H32O5/c1-4-5-6-7-8-11-17-28-24(26)20-13-12-14-21(18-20)25(27)30-23-1

InchiKey: UDBOJJAWJINVCQ-UHFFFAOYSA-N

Formula: C25H32O5

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

Mol. weight [g/mol]: 412.52

Physical Properties

Property code	Value	Unit	Source
gf	-210.10	kJ/mol	Joback Method
hf	-736.31	kJ/mol	Joback Method
hfus	51.05	kJ/mol	Joback Method
hvap	97.45	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.210		Crippen Method
mcvol	336.340	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	3112.00		NIST Webbook
rinpol	3112.00		NIST Webbook
tb	1009.28	K	Joback Method
tc	1238.35	K	Joback Method
tf	600.94	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1103.54	J/mol×K	1009.28	Joback Method
cpg	1116.84	J/mol×K	1047.46	Joback Method
cpg	1128.48	J/mol×K	1085.64	Joback Method
cpg	1138.50	J/mol×K	1123.82	Joback Method
cpg	1146.94	J/mol×K	1162.00	Joback Method
cpg	1153.82	J/mol×K	1200.18	Joback Method
cpg	1159.18	J/mol×K	1238.35	Joback Method
dvisc	0.0002030	Pa×s	600.94	Joback Method

dvisc	0.0001117	Pa×s	669.00	Joback Method
dvisc	0.0000687	Pa×s	737.05	Joback Method
dvisc	0.0000459	Pa×s	805.11	Joback Method
dvisc	0.0000326	Pa×s	873.17	Joback Method
dvisc	0.0000243	Pa×s	941.22	Joback Method
dvisc	0.0000189	Pa×s	1009.28	Joback Method

Sources

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=U344433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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