Isophthalic acid, 2-isopropoxyphenyl dodecyl ester

Inchi: InChI=1S/C29H40O5/c1-4-5-6-7-8-9-10-11-12-15-21-32-28(30)24-17-16-18-25(22-24)29

InchiKey: CPRMJROBVIARDO-UHFFFAOYSA-N

Formula: C29H40O5

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

Mol. weight [g/mol]: 468.62

Physical Properties

Property code	Value	Unit	Source
gf	-176.42	kJ/mol	Joback Method
hf	-818.87	kJ/mol	Joback Method
hfus	61.41	kJ/mol	Joback Method
hvap	106.36	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	7.771		Crippen Method
mcvol	392.700	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	3529.00		NIST Webbook
rinpol	3529.00		NIST Webbook
tb	1100.80	K	Joback Method
tc	1349.52	K	Joback Method
tf	646.02	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.14	J/mol×K	1100.80	Joback Method
cpg	1360.22	J/mol×K	1142.25	Joback Method
cpg	1371.27	J/mol×K	1183.71	Joback Method
cpg	1380.33	J/mol×K	1225.16	Joback Method
cpg	1387.49	J/mol×K	1266.61	Joback Method
cpg	1392.80	J/mol×K	1308.07	Joback Method
cpg	1396.34	J/mol×K	1349.52	Joback Method
dvisc	0.0001237	Pa×s	646.02	Joback Method

dvisc	0.0000656	Pa×s	721.82	Joback Method
dvisc	0.0000393	Pa×s	797.61	Joback Method
dvisc	0.0000257	Pa×s	873.41	Joback Method
dvisc	0.0000180	Pa×s	949.21	Joback Method
dvisc	0.0000133	Pa×s	1025.00	Joback Method
dvisc	0.0000102	Pa×s	1100.80	Joback Method

Sources

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=U344436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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