Isophthalic acid, 2-isopropoxyphenyl undecyl ester

Inchi: InChI=1S/C28H38O5/c1-4-5-6-7-8-9-10-11-14-20-31-27(29)23-16-15-17-24(21-23)28(30
InchiKey: SDHHJYWIJBYNME-UHFFFAOYSA-N
Formula: C28H38O5
SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]: 454.60

Physical Properties

Property code	Value	Unit	Source
gf	-184.84	kJ/mol	Joback Method
hf	-798.23	kJ/mol	Joback Method
hfus	58.82	kJ/mol	Joback Method
hvap	104.13	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	7.381		Crippen Method
mcvol	378.610	ml/mol	McGowan Method
pc	982.08	kPa	Joback Method
rinpol	3421.00		NIST Webbook
rinpol	3421.00		NIST Webbook
tb	1077.92	K	Joback Method
tc	1320.01	K	Joback Method
tf	634.75	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.83	J/mol×K	1077.92	Joback Method
cpg	1298.97	J/mol×K	1118.27	Joback Method
cpg	1310.18	J/mol×K	1158.62	Joback Method
cpg	1319.53	J/mol×K	1198.97	Joback Method
cpg	1327.06	J/mol×K	1239.31	Joback Method
cpg	1332.85	J/mol×K	1279.66	Joback Method
cpg	1336.93	J/mol×K	1320.01	Joback Method
dvisc	0.0001406	Pa×s	634.75	Joback Method

dvisc	0.0000752	Pa×s	708.61	Joback Method
dvisc	0.0000453	Pa×s	782.47	Joback Method
dvisc	0.0000298	Pa×s	856.34	Joback Method
dvisc	0.0000209	Pa×s	930.20	Joback Method
dvisc	0.0000155	Pa×s	1004.06	Joback Method
dvisc	0.0000119	Pa×s	1077.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344435&Units=SI
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

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