Isophthalic acid, 2-isopropoxyphenyl nonyl ester

Inchi: InChI=1S/C26H34O5/c1-4-5-6-7-8-9-12-18-29-25(27)21-14-13-15-22(19-21)26(28)31-24
InchiKey: VTRWEFPEXDTZIN-UHFFFAOYSA-N
Formula: C26H34O5
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]: 426.55

Physical Properties

Property code	Value	Unit	Source
gf	-201.68	kJ/mol	Joback Method
hf	-756.95	kJ/mol	Joback Method
hfus	53.64	kJ/mol	Joback Method
hvap	99.68	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	6.600		Crippen Method
mcvol	350.430	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	1032.16	K	Joback Method
tc	1264.50	K	Joback Method
tf	612.21	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.99	J/mol×K	1032.16	Joback Method
cpg	1213.30	J/mol×K	1225.78	Joback Method
cpg	1206.74	J/mol×K	1187.05	Joback Method
cpg	1198.57	J/mol×K	1148.33	Joback Method
cpg	1188.74	J/mol×K	1109.61	Joback Method
cpg	1177.23	J/mol×K	1070.88	Joback Method
cpg	1218.29	J/mol×K	1264.50	Joback Method
dvisc	0.0000162	Pa×s	1032.16	Joback Method

dvisc	0.0000210	Pa×s	962.17	Joback Method
dvisc	0.0000282	Pa×s	892.18	Joback Method
dvisc	0.0000398	Pa×s	822.18	Joback Method
dvisc	0.0000599	Pa×s	752.19	Joback Method
dvisc	0.0000982	Pa×s	682.20	Joback Method
dvisc	0.0001801	Pa×s	612.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344434&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