Isophthalic acid, decyl 2-isopropylphenyl ester

Inchi: InChI=1S/C27H36O4/c1-4-5-6-7-8-9-10-13-19-30-26(28)22-15-14-16-23(20-22)27(29)31
InchiKey: IBBVJECPUREMSJ-UHFFFAOYSA-N
Formula: C27H36O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-88.26	kJ/mol	Joback Method
hf	-645.37	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	99.50	kJ/mol	Joback Method
log10ws	-8.75		Crippen Method
logp	7.327		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
rinpol	3244.00		NIST Webbook
rinpol	3244.00		NIST Webbook
tb	1032.62	K	Joback Method
tc	1264.92	K	Joback Method
tf	601.25	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1198.18	J/mol×K	1032.62	Joback Method
cpg	1212.63	J/mol×K	1071.34	Joback Method
cpg	1225.49	J/mol×K	1110.05	Joback Method
cpg	1236.84	J/mol×K	1148.77	Joback Method
cpg	1246.72	J/mol×K	1187.49	Joback Method
cpg	1255.22	J/mol×K	1226.20	Joback Method
cpg	1262.38	J/mol×K	1264.92	Joback Method
dvisc	0.0002297	Pa×s	601.25	Joback Method

dvisc	0.0001214	Pa×s	673.14	Joback Method
dvisc	0.0000725	Pa×s	745.04	Joback Method
dvisc	0.0000475	Pa×s	816.93	Joback Method
dvisc	0.0000333	Pa×s	888.83	Joback Method
dvisc	0.0000246	Pa×s	960.72	Joback Method
dvisc	0.0000189	Pa×s	1032.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344639&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

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