Isophthalic acid, dodecyl 2-isopropylphenyl ester

Inchi: InChI=1S/C29H40O4/c1-4-5-6-7-8-9-10-11-12-15-21-32-28(30)24-17-16-18-25(22-24)29

InchiKey: PLVMGQUUSJIIJV-UHFFFAOYSA-N

Formula: C29H40O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1

Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
gf	-71.42	kJ/mol	Joback Method
hf	-686.65	kJ/mol	Joback Method
hfus	60.22	kJ/mol	Joback Method
hvap	103.95	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.107		Crippen Method
mcvol	386.830	ml/mol	McGowan Method
pc	935.20	kPa	Joback Method
rinpol	3450.00		NIST Webbook
rinpol	3450.00		NIST Webbook
tb	1078.38	K	Joback Method
tc	1320.68	K	Joback Method
tf	623.79	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.48	J/mol×K	1078.38	Joback Method
cpg	1336.07	J/mol×K	1118.76	Joback Method
cpg	1348.93	J/mol×K	1159.15	Joback Method
cpg	1360.13	J/mol×K	1199.53	Joback Method
cpg	1369.77	J/mol×K	1239.91	Joback Method
cpg	1377.92	J/mol×K	1280.30	Joback Method
cpg	1384.66	J/mol×K	1320.68	Joback Method
dvisc	0.0001793	Pa×s	623.79	Joback Method

dvisc	0.0000930	Pa×s	699.55	Joback Method
dvisc	0.0000549	Pa×s	775.32	Joback Method
dvisc	0.0000355	Pa×s	851.09	Joback Method
dvisc	0.0000247	Pa×s	926.85	Joback Method
dvisc	0.0000182	Pa×s	1002.62	Joback Method
dvisc	0.0000139	Pa×s	1078.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344641&Units=SI

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