Isophthalic acid, dodecyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C30H48O4/c1-5-6-7-8-9-10-11-12-13-14-22-33-28(31)24-16-15-17-25(23-24)2

InchiKey: VAIVVLATSYGNBV-UHFFFAOYSA-N

Formula: C30H48O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1

Mol. weight [g/mol]: 472.70

Physical Properties

Property code	Value	Unit	Source
gf	-143.76	kJ/mol	Joback Method
hf	-901.84	kJ/mol	Joback Method
hfus	58.17	kJ/mol	Joback Method
hvap	102.45	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.526		Crippen Method
mcvol	413.820	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	3548.00		NIST Webbook
rinpol	3548.00		NIST Webbook
tb	1081.69	K	Joback Method
tc	1325.22	K	Joback Method
tf	616.68	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1494.16	J/mol×K	1081.69	Joback Method
cpg	1560.25	J/mol×K	1284.63	Joback Method
cpg	1550.51	J/mol×K	1244.04	Joback Method
cpg	1539.15	J/mol×K	1203.45	Joback Method
cpg	1526.04	J/mol×K	1162.87	Joback Method
cpg	1511.08	J/mol×K	1122.28	Joback Method
cpg	1568.47	J/mol×K	1325.22	Joback Method
dvisc	0.0000127	Pa×s	1081.69	Joback Method

dvisc	0.0000168	Pa×s	1004.19	Joback Method
dvisc	0.0000234	Pa×s	926.69	Joback Method
dvisc	0.0000346	Pa×s	849.18	Joback Method
dvisc	0.0000554	Pa×s	771.68	Joback Method
dvisc	0.0000983	Pa×s	694.18	Joback Method
dvisc	0.0002018	Pa×s	616.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345743&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