Isophthalic acid, isohexyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C24H36O4/c1-17(2)8-7-15-27-22(25)18-9-6-10-19(16-18)23(26)28-21-13-11-2

InchiKey: PJJYXCZBSBYVKT-UHFFFAOYSA-N

Formula: C24H36O4

SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-196.72	kJ/mol	Joback Method
hf	-783.28	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.041		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2867.00		NIST Webbook
rinpol	2867.00		NIST Webbook
tb	943.97	K	Joback Method
tc	1169.10	K	Joback Method
tf	534.06	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.51	J/mol×K	943.97	Joback Method
cpg	1136.81	J/mol×K	981.49	Joback Method
cpg	1152.43	J/mol×K	1019.01	Joback Method
cpg	1166.43	J/mol×K	1056.53	Joback Method
cpg	1178.87	J/mol×K	1094.05	Joback Method
cpg	1189.81	J/mol×K	1131.57	Joback Method
cpg	1199.33	J/mol×K	1169.10	Joback Method
dvisc	0.0004832	Pa×s	534.06	Joback Method

dvisc	0.0002326	Pa×s	602.38	Joback Method
dvisc	0.0001299	Pa×s	670.70	Joback Method
dvisc	0.0000808	Pa×s	739.01	Joback Method
dvisc	0.0000545	Pa×s	807.33	Joback Method
dvisc	0.0000391	Pa×s	875.65	Joback Method
dvisc	0.0000294	Pa×s	943.97	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=U345737&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