Isophthalic acid, hexyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C24H36O4/c1-5-6-7-8-16-27-22(25)18-10-9-11-19(17-18)23(26)28-21-14-12-2

InchiKey: OFGIUXAZAVUZFD-UHFFFAOYSA-N

Formula: C24H36O4

SMILES: CCCCCCOC(=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	-194.28	kJ/mol	Joback Method
hf	-778.00	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	89.09	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.185		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2916.00		NIST Webbook
rinpol	2916.00		NIST Webbook
tb	944.41	K	Joback Method
tc	1167.67	K	Joback Method
tf	549.06	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.09	J/mol×K	944.41	Joback Method
cpg	1136.30	J/mol×K	981.62	Joback Method
cpg	1151.86	J/mol×K	1018.83	Joback Method
cpg	1165.84	J/mol×K	1056.04	Joback Method
cpg	1178.30	J/mol×K	1093.25	Joback Method
cpg	1189.31	J/mol×K	1130.46	Joback Method
cpg	1198.92	J/mol×K	1167.67	Joback Method
dvisc	0.0004325	Pa×s	549.06	Joback Method

dvisc	0.0002225	Pa×s	614.95	Joback Method
dvisc	0.0001302	Pa×s	680.84	Joback Method
dvisc	0.0000837	Pa×s	746.73	Joback Method
dvisc	0.0000578	Pa×s	812.63	Joback Method
dvisc	0.0000422	Pa×s	878.52	Joback Method
dvisc	0.0000322	Pa×s	944.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345738&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