Isophthalic acid, nonyl 4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C27H42O4/c1-5-6-7-8-9-10-11-19-30-25(28)21-13-12-14-22(20-21)26(29)31-2
InchiKey: SHJCJMZDTBDSCM-UHFFFAOYSA-N
Formula: C27H42O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-169.02	kJ/mol	Joback Method
hf	-839.92	kJ/mol	Joback Method
hfus	50.40	kJ/mol	Joback Method
hvap	95.77	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.356		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	3233.00		NIST Webbook
rinpol	3233.00		NIST Webbook
tb	1013.05	K	Joback Method
tc	1241.89	K	Joback Method
tf	582.87	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.17	J/mol×K	1013.05	Joback Method
cpg	1373.10	J/mol×K	1203.75	Joback Method
cpg	1362.70	J/mol×K	1165.61	Joback Method
cpg	1350.79	J/mol×K	1127.47	Joback Method
cpg	1337.28	J/mol×K	1089.33	Joback Method
cpg	1322.10	J/mol×K	1051.19	Joback Method
cpg	1382.07	J/mol×K	1241.89	Joback Method
dvisc	0.0000203	Pa×s	1013.05	Joback Method

dvisc	0.0000268	Pa×s	941.35	Joback Method
dvisc	0.0000371	Pa×s	869.66	Joback Method
dvisc	0.0000543	Pa×s	797.96	Joback Method
dvisc	0.0000857	Pa×s	726.26	Joback Method
dvisc	0.0001494	Pa×s	654.57	Joback Method
dvisc	0.0002989	Pa×s	582.87	Joback Method

Sources

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=U345741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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