Phthalic acid, isohexyl 2-tert-butyl-6-methylphenyl ester

Inchi: InChI=1S/C25H32O4/c1-17(2)11-10-16-28-23(26)19-13-7-8-14-20(19)24(27)29-22-18(3)

InchiKey: YNRWOVREAWBHCV-UHFFFAOYSA-N

Formula: C25H32O4

SMILES: Cc1cccc(C(C)(C)C)c1OC(=O)c1ccccc1C(=O)OCCCC(C)C

Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-111.89	kJ/mol	Joback Method
hf	-624.31	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	94.41	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.105		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	2687.00		NIST Webbook
tb	988.61	K	Joback Method
tc	1219.80	K	Joback Method
tf	593.65	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.53	J/mol×K	988.61	Joback Method
cpg	1090.05	J/mol×K	1027.14	Joback Method
cpg	1103.17	J/mol×K	1065.67	Joback Method
cpg	1114.93	J/mol×K	1104.20	Joback Method
cpg	1125.42	J/mol×K	1142.74	Joback Method
cpg	1134.70	J/mol×K	1181.27	Joback Method
cpg	1142.85	J/mol×K	1219.80	Joback Method
dvisc	0.0002224	Pa×s	593.65	Joback Method
dvisc	0.0001216	Pa×s	659.48	Joback Method

dvisc	0.0000742	Pa×s	725.30	Joback Method
dvisc	0.0000491	Pa×s	791.13	Joback Method
dvisc	0.0000347	Pa×s	856.96	Joback Method
dvisc	0.0000257	Pa×s	922.78	Joback Method
dvisc	0.0000198	Pa×s	988.61	Joback Method

Sources

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=U357096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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