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

Inchi: InChI=1S/C25H32O4/c1-6-7-8-11-17-28-23(26)19-14-9-10-15-20(19)24(27)29-22-18(2)1

InchiKey: RPIODNAHQRKMFV-UHFFFAOYSA-N

Formula: C25H32O4

SMILES: CCCCCCOC(=O)c1ccccc1C(=O)Oc1c(C)cccc1C(C)(C)C

Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-109.45	kJ/mol	Joback Method
hf	-619.03	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	94.80	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.249		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2733.00		NIST Webbook
tb	989.05	K	Joback Method
tc	1218.67	K	Joback Method
tf	608.65	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.14	J/mol×K	989.05	Joback Method
cpg	1089.64	J/mol×K	1027.32	Joback Method
cpg	1102.75	J/mol×K	1065.59	Joback Method
cpg	1114.55	J/mol×K	1103.86	Joback Method
cpg	1125.10	J/mol×K	1142.13	Joback Method
cpg	1134.48	J/mol×K	1180.40	Joback Method
cpg	1142.76	J/mol×K	1218.67	Joback Method
dvisc	0.0002059	Pa×s	608.65	Joback Method
dvisc	0.0001187	Pa×s	672.05	Joback Method

dvisc	0.0000752	Pa×s	735.45	Joback Method
dvisc	0.0000513	Pa×s	798.85	Joback Method
dvisc	0.0000370	Pa×s	862.25	Joback Method
dvisc	0.0000279	Pa×s	925.65	Joback Method
dvisc	0.0000218	Pa×s	989.05	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=U357097&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