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

Inchi: InChI=1S/C27H36O4/c1-6-7-8-9-10-13-19-30-25(28)21-16-11-12-17-22(21)26(29)31-24-

InchiKey: CGGZLIMNNFRERI-UHFFFAOYSA-N

Formula: C27H36O4

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

Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-92.61	kJ/mol	Joback Method
hf	-660.31	kJ/mol	Joback Method
hfus	50.76	kJ/mol	Joback Method
hvap	99.25	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.029		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
rinpol	2926.00		NIST Webbook
rinpol	2926.00		NIST Webbook
tb	1034.81	K	Joback Method
tc	1268.75	K	Joback Method
tf	631.19	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1196.97	J/mol×K	1034.81	Joback Method
cpg	1256.51	J/mol×K	1229.76	Joback Method
cpg	1247.17	J/mol×K	1190.77	Joback Method
cpg	1236.63	J/mol×K	1151.78	Joback Method
cpg	1224.80	J/mol×K	1112.79	Joback Method
cpg	1211.61	J/mol×K	1073.80	Joback Method
cpg	1264.74	J/mol×K	1268.75	Joback Method
dvisc	0.0000160	Pa×s	1034.81	Joback Method

dvisc	0.0000206	Pa×s	967.54	Joback Method
dvisc	0.0000275	Pa×s	900.27	Joback Method
dvisc	0.0000385	Pa×s	833.00	Joback Method
dvisc	0.0000571	Pa×s	765.73	Joback Method
dvisc	0.0000915	Pa×s	698.46	Joback Method
dvisc	0.0001620	Pa×s	631.19	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=U357098&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