Bis(4-tert-butyl-2-methylphenyl) phthalate

Inchi: InChI=1S/C30H34O4/c1-19-17-21(29(3,4)5)13-15-25(19)33-27(31)23-11-9-10-12-24(23)
InchiKey: JIQXNNGUGZEDSN-UHFFFAOYSA-N
Formula: C30H34O4
SMILES: Cc1cc(C(C)(C)C)ccc1OC(=O)c1ccccc1C(=O)Oc1ccc(C(C)(C)C)cc1C
Mol. weight [g/mol]: 458.59
CAS: 116595-13-2

Physical Properties

Property code	Value	Unit	Source
gf	28.64	kJ/mol	Joback Method
hf	-517.39	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	108.23	kJ/mol	Joback Method
log10ws	-9.22		Crippen Method
logp	7.337		Crippen Method
mcvol	377.160	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
tb	1136.86	K	Joback Method
tc	1396.16	K	Joback Method
tf	718.88	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1264.25	J/mol×K	1136.86	Joback Method
cpg	1316.10	J/mol×K	1352.94	Joback Method
cpg	1307.65	J/mol×K	1309.73	Joback Method
cpg	1298.40	J/mol×K	1266.51	Joback Method
cpg	1288.18	J/mol×K	1223.29	Joback Method
cpg	1276.85	J/mol×K	1180.08	Joback Method
cpg	1323.88	J/mol×K	1396.16	Joback Method
dvisc	0.0000082	Pa×s	1136.86	Joback Method
dvisc	0.0000104	Pa×s	1067.20	Joback Method

dvisc	0.0000137	Pa×s	997.53	Joback Method
dvisc	0.0000187	Pa×s	927.87	Joback Method
dvisc	0.0000271	Pa×s	858.21	Joback Method
dvisc	0.0000417	Pa×s	788.54	Joback Method
dvisc	0.0000698	Pa×s	718.88	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=C116595132&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume