

2,4-Di-tert-butyl-6-chlorophenyl benzoate

Inchi:	InChI=1S/C21H25ClO2/c1-20(2,3)15-12-16(21(4,5)6)18(17(22)13-15)24-19(23)14-10-8-7
InchiKey:	KMADBTvKBVDACU-UHFFFAOYSA-N
Formula:	C21H25ClO2
SMILES:	CC(C)(C)c1cc(Cl)c(OC(=O)c2ccccc2)c(C(C)(C)C)c1
Mol. weight [g/mol]:	344.88
CAS:	116632-94-1

Physical Properties

Property code	Value	Unit	Source
gf	81.70	kJ/mol	Joback Method
hf	-316.16	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.154		Crippen Method
mcvol	278.910	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
tb	855.44	K	Joback Method
tc	1095.89	K	Joback Method
tf	523.75	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.76	J/molxK	855.44	Joback Method
cpg	838.90	J/molxK	895.51	Joback Method
cpg	853.77	J/molxK	935.59	Joback Method
cpg	867.48	J/molxK	975.66	Joback Method
cpg	880.15	J/molxK	1015.74	Joback Method
cpg	891.89	J/molxK	1055.81	Joback Method
cpg	902.82	J/molxK	1095.89	Joback Method
dvisc	0.0004049	Paxs	523.75	Joback Method
dvisc	0.0002251	Paxs	579.03	Joback Method

dvisc	0.0001386	Paxs	634.31	Joback Method
dvisc	0.0000922	Paxs	689.60	Joback Method
dvisc	0.0000652	Paxs	744.88	Joback Method
dvisc	0.0000484	Paxs	800.16	Joback Method
dvisc	0.0000373	Paxs	855.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116632941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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