

# 4-(1,1-Dimethylhexyl)phenyl 4-chlorobenzoate

<b>Inchi:</b>	InChI=1S/C21H25ClO2/c1-4-5-6-15-21(2,3)17-9-13-19(14-10-17)24-20(23)16-7-11-18(22)
<b>InchiKey:</b>	DUUQPFSNLIDLXZ-UHFFFAOYSA-N
<b>Formula:</b>	C21H25ClO2
<b>SMILES:</b>	CCCCC(C)(C)c1ccc(OC(=O)c2ccc(Cl)cc2)cc1
<b>Mol. weight [g/mol]:</b>	344.88

## Physical Properties

Property code	Value	Unit	Source
gf	88.49	kJ/mol	Joback Method
hf	-295.94	kJ/mol	Joback Method
hfus	37.02	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.417		Crippen Method
mcvol	278.910	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
tb	853.69	K	Joback Method
tc	1083.40	K	Joback Method
tf	508.81	K	Joback Method
vc	1.058	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.65	J/molxK	853.69	Joback Method
cpg	890.43	J/molxK	1045.11	Joback Method
cpg	879.00	J/molxK	1006.83	Joback Method
cpg	866.60	J/molxK	968.54	Joback Method
cpg	853.13	J/molxK	930.26	Joback Method
cpg	838.51	J/molxK	891.97	Joback Method
cpg	900.97	J/molxK	1083.40	Joback Method
dvisc	0.0000467	Paxs	853.69	Joback Method
dvisc	0.0000604	Paxs	796.21	Joback Method
dvisc	0.0000812	Paxs	738.73	Joback Method

dvisc	0.0001149	Paxs	681.25	Joback Method
dvisc	0.0001731	Paxs	623.77	Joback Method
dvisc	0.0002835	Paxs	566.29	Joback Method
dvisc	0.0005192	Paxs	508.81	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004130&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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