

# 4-(4-Chloro-2-methylphenoxy)butyric acid, hexyl ester

Inchi:	InChI=1S/C17H25ClO3/c1-3-4-5-6-11-21-17(19)8-7-12-20-16-10-9-15(18)13-14(16)2/h9-
InchiKey:	YLJLRVKCBMBORZ-UHFFFAOYSA-N
Formula:	C17H25ClO3
SMILES:	CCCCCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]:	312.83

## Physical Properties

Property code	Value	Unit	Source
gf	-165.44	kJ/mol	Joback Method
hf	-573.38	kJ/mol	Joback Method
hfus	41.22	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.931		Crippen Method
mvol	252.180	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2795.00		NIST Webbook
rinpol	2795.00		NIST Webbook
tb	761.14	K	Joback Method
tc	959.53	K	Joback Method
tf	457.12	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.02	J/molxK	761.14	Joback Method
cpg	728.84	J/molxK	794.20	Joback Method
cpg	743.69	J/molxK	827.27	Joback Method
cpg	757.59	J/molxK	860.33	Joback Method
cpg	770.54	J/molxK	893.40	Joback Method
cpg	782.57	J/molxK	926.46	Joback Method
cpg	793.69	J/molxK	959.53	Joback Method
dvisc	0.0006654	Paxs	457.12	Joback Method

dvisc	0.0003852	Paxs	507.79	Joback Method
dvisc	0.0002463	Paxs	558.46	Joback Method
dvisc	0.0001696	Paxs	609.13	Joback Method
dvisc	0.0001237	Paxs	659.80	Joback Method
dvisc	0.0000944	Paxs	710.47	Joback Method
dvisc	0.0000746	Paxs	761.14	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415082&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415082&amp;Units=SI</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>rinpol:</b>	Non-polar retention indices
<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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