

# Phenylacetic acid, 2-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C14H11ClO2/c15-12-8-4-5-9-13(12)17-14(16)10-11-6-2-1-3-7-11/h1-9H,10H2
<b>InchiKey:</b>	KQBWWQRVHFNTSK-UHFFFAOYSA-N
<b>Formula:</b>	C14H11ClO2
<b>SMILES:</b>	O=C(Cc1ccccc1)Oc1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	246.69

## Physical Properties

Property code	Value	Unit	Source
gf	36.34	kJ/mol	Joback Method
hf	-131.24	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	65.51	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.488		Crippen Method
mvol	180.280	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	691.78	K	Joback Method
tc	938.00	K	Joback Method
tf	414.98	K	Joback Method
vc	0.676	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.76	J/molxK	691.78	Joback Method
cpg	453.56	J/molxK	732.82	Joback Method
cpg	466.19	J/molxK	773.85	Joback Method
cpg	477.72	J/molxK	814.89	Joback Method
cpg	488.18	J/molxK	855.92	Joback Method
cpg	497.64	J/molxK	896.96	Joback Method
cpg	506.14	J/molxK	938.00	Joback Method
dvisc	0.0011566	Paxs	414.98	Joback Method

dvisc	0.0006831	Paxs	461.11	Joback Method
dvisc	0.0004441	Paxs	507.25	Joback Method
dvisc	0.0003102	Paxs	553.38	Joback Method
dvisc	0.0002289	Paxs	599.51	Joback Method
dvisc	0.0001765	Paxs	645.65	Joback Method
dvisc	0.0001408	Paxs	691.78	Joback Method

## Sources

<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=U299005&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299005&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>

## 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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