

# Phenylacetic acid, 4-chloro-, octyl ester

<b>Inchi:</b>	InChI=1S/C16H23ClO2/c1-2-3-4-5-6-7-12-19-16(18)13-14-8-10-15(17)11-9-14/h8-11H,2
<b>InchiKey:</b>	KXKWBFXGXVAMQO-UHFFFAOYSA-N
<b>Formula:</b>	C16H23ClO2
<b>SMILES:</b>	CCCCCCCCOC(=O)Cc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	282.81

## Physical Properties

Property code	Value	Unit	Source
gf	-59.23	kJ/mol	Joback Method
hf	-409.05	kJ/mol	Joback Method
hfus	37.83	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.786		Crippen Method
mvol	232.220	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	710.86	K	Joback Method
tc	910.76	K	Joback Method
tf	411.10	K	Joback Method
vc	0.896	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.76	J/molxK	710.86	Joback Method
cpg	645.71	J/molxK	744.18	Joback Method
cpg	660.72	J/molxK	777.49	Joback Method
cpg	674.83	J/molxK	810.81	Joback Method
cpg	688.05	J/molxK	844.12	Joback Method
cpg	700.42	J/molxK	877.44	Joback Method
cpg	711.96	J/molxK	910.76	Joback Method
dvisc	0.0012148	Paxs	411.10	Joback Method

dvisc	0.0006558	Paxs	461.06	Joback Method
dvisc	0.0003994	Paxs	511.02	Joback Method
dvisc	0.0002657	Paxs	560.98	Joback Method
dvisc	0.0001889	Paxs	610.94	Joback Method
dvisc	0.0001415	Paxs	660.90	Joback Method
dvisc	0.0001103	Paxs	710.86	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406212&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>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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