

# (4-Chloro-2-methylphenoxy)acetic acid, pentafluorobenzyl ester

Other names:	MCPA, PFB MCPA PFB ester
Inchi:	InChI=1S/C16H10ClF5O3/c1-7-4-8(17)2-3-10(7)24-6-11(23)25-5-9-12(18)14(20)16(22)1
InchiKey:	SXGAQQYJZZFKIY-UHFFFAOYSA-N
Formula:	C16H10ClF5O3
SMILES:	<chem>Cc1cc(Cl)ccc1OCC(=O)OCc1c(F)c(F)c(F)c(F)c1F</chem>
Mol. weight [g/mol]:	380.69
CAS:	61443-55-8

## Physical Properties

Property code	Value	Unit	Source
gf	-1083.65	kJ/mol	Joback Method
hf	-1354.11	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.466		Crippen Method
mvol	223.180	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	2015.00		NIST Webbook
ripol	2820.00		NIST Webbook
ripol	2852.00		NIST Webbook
ripol	2819.00		NIST Webbook
ripol	2819.00		NIST Webbook
tb	786.19	K	Joback Method
tc	986.08	K	Joback Method
tf	537.82	K	Joback Method
vc	0.896	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	600.36	J/mol×K	786.19	Joback Method
cpg	611.26	J/mol×K	819.50	Joback Method
cpg	621.35	J/mol×K	852.82	Joback Method
cpg	630.63	J/mol×K	886.13	Joback Method
cpg	639.08	J/mol×K	919.45	Joback Method
cpg	646.71	J/mol×K	952.76	Joback Method
cpg	653.50	J/mol×K	986.08	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=C61443558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61443558&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>ripol:</b>	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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