

# (2,4,5-Trichlorophenoxy)acetic acid, sec-butyl ester

Inchi:	InChI=1S/C12H13Cl3O3/c1-3-7(2)18-12(16)6-17-11-5-9(14)8(13)4-10(11)15/h4-5,7H,3,6
InchiKey:	KOCPUBZALOBLTB-UHFFFAOYSA-N
Formula:	C12H13Cl3O3
SMILES:	CCC(C)OC(=O)COc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	311.59
CAS:	61792-07-2

## Physical Properties

Property code	Value	Unit	Source
gf	-243.47	kJ/mol	Joback Method
hf	-518.41	kJ/mol	Joback Method
hfus	32.75	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.367		Crippen Method
mcvol	206.210	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
tb	726.14	K	Joback Method
tc	946.85	K	Joback Method
tf	458.13	K	Joback Method
vc	0.782	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.15	J/molxK	726.14	Joback Method
cpg	544.92	J/molxK	910.07	Joback Method
cpg	536.43	J/molxK	873.28	Joback Method
cpg	527.10	J/molxK	836.50	Joback Method
cpg	516.94	J/molxK	799.71	Joback Method
cpg	505.96	J/molxK	762.93	Joback Method
cpg	552.57	J/molxK	946.85	Joback Method
dvisc	0.0001035	Paxs	726.14	Joback Method
dvisc	0.0001281	Paxs	681.47	Joback Method

dvisc	0.0001633	Paxs	636.80	Joback Method
dvisc	0.0002160	Paxs	592.13	Joback Method
dvisc	0.0002991	Paxs	547.47	Joback Method
dvisc	0.0004389	Paxs	502.80	Joback Method
dvisc	0.0006939	Paxs	458.13	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C61792072&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61792072&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>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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