

# 6-Methylheptyl (2,4,5-trichlorophenoxy)acetate

<b>Inchi:</b>	InChI=1S/C16H21Cl3O3/c1-11(2)6-4-3-5-7-21-16(20)10-22-15-9-13(18)12(17)8-14(15)19
<b>InchiKey:</b>	LRDPQMJVRJVAOH-UHFFFAOYSA-N
<b>Formula:</b>	C16H21Cl3O3
<b>SMILES:</b>	CC(C)CCCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	367.69
<b>CAS:</b>	116436-47-6

## Physical Properties

Property code	Value	Unit	Source
gf	-209.79	kJ/mol	Joback Method
hf	-600.97	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.785		Crippen Method
mcvol	262.570	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
tb	817.66	K	Joback Method
tc	1028.55	K	Joback Method
tf	503.21	K	Joback Method
vc	1.006	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.62	J/molxK	817.66	Joback Method
cpg	723.04	J/molxK	852.81	Joback Method
cpg	735.46	J/molxK	887.96	Joback Method
cpg	746.89	J/molxK	923.11	Joback Method
cpg	757.34	J/molxK	958.26	Joback Method
cpg	766.83	J/molxK	993.40	Joback Method
cpg	775.36	J/molxK	1028.55	Joback Method
dvisc	0.0004920	Paxs	503.21	Joback Method
dvisc	0.0002944	Paxs	555.62	Joback Method

dvisc	0.0001925	Paxs	608.03	Joback Method
dvisc	0.0001347	Paxs	660.43	Joback Method
dvisc	0.0000993	Paxs	712.84	Joback Method
dvisc	0.0000763	Paxs	765.25	Joback Method
dvisc	0.0000607	Paxs	817.66	Joback Method

## Sources

<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=C116436476&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436476&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>

## 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>mccvol:</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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