

# Heptyl 2,4,5-trichlorophenyl ether

<b>Inchi:</b>	InChI=1S/C13H17Cl3O/c1-2-3-4-5-6-7-17-13-9-11(15)10(14)8-12(13)16/h8-9H,2-7H2,1H
<b>InchiKey:</b>	PUMPSSGWRRHJN-UHFFFAOYSA-N
<b>Formula:</b>	C13H17Cl3O
<b>SMILES:</b>	CCCCCCCOc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	295.63
<b>CAS:</b>	116401-40-2

## Physical Properties

Property code	Value	Unit	Source
gf	1.31	kJ/mol	Joback Method
hf	-288.97	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.996		Crippen Method
mcvol	212.860	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
tb	673.17	K	Joback Method
tc	882.88	K	Joback Method
tf	412.24	K	Joback Method
vc	0.821	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.25	J/molxK	673.17	Joback Method
cpg	520.00	J/molxK	708.12	Joback Method
cpg	532.96	J/molxK	743.07	Joback Method
cpg	545.15	J/molxK	778.02	Joback Method
cpg	556.58	J/molxK	812.98	Joback Method
cpg	567.28	J/molxK	847.93	Joback Method
cpg	577.26	J/molxK	882.88	Joback Method
dvisc	0.0008792	Paxs	412.24	Joback Method
dvisc	0.0005470	Paxs	455.73	Joback Method

dvisc	0.0003696	Paxs	499.22	Joback Method
dvisc	0.0002660	Paxs	542.71	Joback Method
dvisc	0.0002010	Paxs	586.19	Joback Method
dvisc	0.0001578	Paxs	629.68	Joback Method
dvisc	0.0001279	Paxs	673.17	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401402&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401402&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>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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