

# 2-Phenoxyethyl nonanoate

Inchi:

InChI=1S/C17H26O3/c1-2-3-4-5-6-10-13-17(18)20-15-14-19-16-11-8-7-9-12-16/h7-9,11-

InchiKey:

AIBGEXLVFNCYTE-UHFFFAOYSA-N

Formula:

C17H26O3

SMILES:

CCCCCCCCC(=O)OCCOc1ccccc1

Mol. weight [g/mol]:

278.39

## Physical Properties

Property code	Value	Unit	Source
gf	-134.25	kJ/mol	Joback Method
hf	-534.70	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	67.28	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.359		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	713.75	K	Joback Method
tc	906.43	K	Joback Method
tf	402.16	K	Joback Method
vc	0.921	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.15	J/molxK	713.75	Joback Method
cpg	760.14	J/molxK	874.32	Joback Method
cpg	746.81	J/molxK	842.20	Joback Method
cpg	732.57	J/molxK	810.09	Joback Method
cpg	717.39	J/molxK	777.98	Joback Method
cpg	701.25	J/molxK	745.86	Joback Method
cpg	772.57	J/molxK	906.43	Joback Method
dvisc	0.0000834	Paxs	713.75	Joback Method
dvisc	0.0001090	Paxs	661.82	Joback Method

dvisc	0.0001492	Paxs	609.89	Joback Method
dvisc	0.0002163	Paxs	557.96	Joback Method
dvisc	0.0003385	Paxs	506.02	Joback Method
dvisc	0.0005869	Paxs	454.09	Joback Method
dvisc	0.0011729	Paxs	402.16	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=R540846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R540846&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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