

# Isoheptadecanol

<b>Inchi:</b>	InChI=1S/C17H36O/c1-17(2)15-13-11-9-7-5-3-4-6-8-10-12-14-16-18/h17-18H,3-16H2,1-
<b>InchiKey:</b>	VWIXGTHYBZXAPS-UHFFFAOYSA-N
<b>Formula:</b>	C17H36O
<b>SMILES:</b>	CC(C)CCCCCCCCCCCCCO
<b>Mol. weight [g/mol]:</b>	256.47
<b>CAS:</b>	57289-07-3

## Physical Properties

Property code	Value	Unit	Source
gf	-47.00	kJ/mol	Joback Method
hf	-551.72	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.706		Crippen Method
mcvol	256.260	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
ripol	2415.00		NIST Webbook
ripol	2415.00		NIST Webbook
tb	680.10	K	Joback Method
tc	842.79	K	Joback Method
tf	327.17	K	Joback Method
vc	1.000	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.91	J/molxK	680.10	Joback Method
cpg	767.57	J/molxK	707.21	Joback Method
cpg	784.49	J/molxK	734.33	Joback Method
cpg	800.68	J/molxK	761.44	Joback Method
cpg	816.17	J/molxK	788.56	Joback Method
cpg	830.98	J/molxK	815.67	Joback Method
cpg	845.14	J/molxK	842.79	Joback Method

dvisc	0.0107169	Paxs	327.17	Joback Method
dvisc	0.0019407	Paxs	385.99	Joback Method
dvisc	0.0005522	Paxs	444.81	Joback Method
dvisc	0.0002108	Paxs	503.63	Joback Method
dvisc	0.0000984	Paxs	562.46	Joback Method
dvisc	0.0000531	Paxs	621.28	Joback Method
dvisc	0.0000318	Paxs	680.10	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=C57289073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57289073&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307i">http://pubs.acs.org/doi/abs/10.1021/ci990307i</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>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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