

# Isobutyl triacontyl ether

**Inchi:** InChI=1S/C34H70O/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26  
**InchiKey:** TUPBYXJOEZVCLM-UHFFFAOYSA-N  
**Formula:** C34H70O  
**SMILES:** CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCC(C)C  
**Mol. weight [g/mol]:** 494.92

## Physical Properties

Property code	Value	Unit	Source
gf	127.96	kJ/mol	Joback Method
hf	-882.59	kJ/mol	Joback Method
hfus	81.48	kJ/mol	Joback Method
hvap	93.30	kJ/mol	Joback Method
log10ws	-12.90		Crippen Method
logp	12.602		Crippen Method
mcvol	495.790	ml/mol	McGowan Method
pc	495.81	kPa	Joback Method
rinpol	3419.00		NIST Webbook
rinpol	3419.00		NIST Webbook
tb	999.30	K	Joback Method
tc	1263.01	K	Joback Method
tf	480.17	K	Joback Method
vc	1.952	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1791.93	J/molxK	999.30	Joback Method
cpg	1823.82	J/molxK	1043.25	Joback Method
cpg	1853.16	J/molxK	1087.20	Joback Method
cpg	1880.12	J/molxK	1131.15	Joback Method
cpg	1904.88	J/molxK	1175.11	Joback Method
cpg	1927.60	J/molxK	1219.06	Joback Method
cpg	1948.47	J/molxK	1263.01	Joback Method
dvisc	0.0004635	Paxs	480.17	Joback Method

dvisc	0.0001442	Paxs	566.69	Joback Method
dvisc	0.0000611	Paxs	653.21	Joback Method
dvisc	0.0000317	Paxs	739.73	Joback Method
dvisc	0.0000188	Paxs	826.26	Joback Method
dvisc	0.0000124	Paxs	912.78	Joback Method
dvisc	0.0000087	Paxs	999.30	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406335&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406335&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>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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