

# Isobutyl pentadecanoate

<b>Inchi:</b>	InChI=1S/C19H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19(20)21-17-18(2)3/h18H,4-
<b>InchiKey:</b>	ACTVSSLKFXCSBT-UHFFFAOYSA-N
<b>Formula:</b>	C19H38O2
<b>SMILES:</b>	CCCCCCCCCCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	298.50

## Physical Properties

Property code	Value	Unit	Source
gf	-127.26	kJ/mol	Joback Method
hf	-685.57	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	6.277		Crippen Method
mvol	286.010	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	709.97	K	Joback Method
tc	880.96	K	Joback Method
tf	361.05	K	Joback Method
vc	1.117	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.12	J/molxK	709.97	Joback Method
cpg	868.53	J/molxK	738.47	Joback Method
cpg	887.04	J/molxK	766.97	Joback Method
cpg	904.69	J/molxK	795.46	Joback Method
cpg	921.48	J/molxK	823.96	Joback Method
cpg	937.44	J/molxK	852.46	Joback Method
cpg	952.60	J/molxK	880.96	Joback Method
dvisc	0.0023450	Paxs	361.05	Joback Method

dvisc	0.0008954	Paxs	419.20	Joback Method
dvisc	0.0004323	Paxs	477.36	Joback Method
dvisc	0.0002445	Paxs	535.51	Joback Method
dvisc	0.0001546	Paxs	593.66	Joback Method
dvisc	0.0001061	Paxs	651.82	Joback Method
dvisc	0.0000774	Paxs	709.97	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R543390&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R543390&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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