

# Octatriacontane, 3-methyl-

Inchi:

InChI=1S/C39H80/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-2

InchiKey:

YXAAQQSWGJSABO-UHFFFAOYSA-N

Formula:

C39H80

SMILES:

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CC

Mol. weight [g/mol]:

549.05

## Physical Properties

Property code	Value	Unit	Source
gf	275.06	kJ/mol	Joback Method
hf	-853.57	kJ/mol	Joback Method
hfus	93.24	kJ/mol	Joback Method
hvap	102.02	kJ/mol	Joback Method
log10ws	-15.91		Crippen Method
logp	15.316		Crippen Method
mcvol	560.370	ml/mol	McGowan Method
pc	407.46	kPa	Joback Method
rinpol	3870.00		NIST Webbook
tb	1091.28	K	Joback Method
tc	1435.32	K	Joback Method
tf	514.29	K	Joback Method
vc	2.213	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.47	J/molxK	1091.28	Joback Method
cpg	2146.26	J/molxK	1148.62	Joback Method
cpg	2183.49	J/molxK	1205.96	Joback Method
cpg	2217.67	J/molxK	1263.30	Joback Method
cpg	2249.30	J/molxK	1320.64	Joback Method
cpg	2278.91	J/molxK	1377.98	Joback Method
cpg	2306.99	J/molxK	1435.32	Joback Method
dvisc	0.0003317	Paxs	514.29	Joback Method
dvisc	0.0000968	Paxs	610.45	Joback Method

dvisc	0.0000395	Paxs	706.62	Joback Method
dvisc	0.0000200	Paxs	802.78	Joback Method
dvisc	0.0000117	Paxs	898.95	Joback Method
dvisc	0.0000076	Paxs	995.12	Joback Method
dvisc	0.0000053	Paxs	1091.28	Joback Method

## Sources

<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=R283682&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R283682&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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