

# (S)13,25-dimethyl-heptatriacontane

<b>Inchi:</b>	InChI=1S/C39H80/c1-5-7-9-11-13-15-18-22-26-30-34-38(3)36-32-28-24-20-17-21-25-29
<b>InchiKey:</b>	PBKCVRRCPRBQIFG-LJEWAXOPSA-N
<b>Formula:</b>	C39H80
<b>SMILES:</b>	CCCCCCCCCCCC(C)CCCCCCCCCCCC(C)CCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	549.05

## Physical Properties

Property code	Value	Unit	Source
gf	272.62	kJ/mol	Joback Method
hf	-858.85	kJ/mol	Joback Method
hfus	89.72	kJ/mol	Joback Method
hvap	101.63	kJ/mol	Joback Method
log10ws	-15.66		Crippen Method
logp	15.172		Crippen Method
mvol	560.370	ml/mol	McGowan Method
pc	408.78	kPa	Joback Method
rinpol	3763.00		NIST Webbook
rinpol	3763.00		NIST Webbook
tb	1090.84	K	Joback Method
tc	1428.32	K	Joback Method
tf	499.29	K	Joback Method
vc	2.208	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2105.46	J/molxK	1090.84	Joback Method
cpg	2145.37	J/molxK	1147.09	Joback Method
cpg	2181.80	J/molxK	1203.33	Joback Method
cpg	2215.23	J/molxK	1259.58	Joback Method
cpg	2246.16	J/molxK	1315.83	Joback Method
cpg	2275.06	J/molxK	1372.07	Joback Method
cpg	2302.42	J/molxK	1428.32	Joback Method
dvisc	0.0003958	Paxs	499.29	Joback Method

dvisc	0.0001036	Paxs	597.88	Joback Method
dvisc	0.0000396	Paxs	696.47	Joback Method
dvisc	0.0000192	Paxs	795.06	Joback Method
dvisc	0.0000110	Paxs	893.66	Joback Method
dvisc	0.0000070	Paxs	992.25	Joback Method
dvisc	0.0000048	Paxs	1090.84	Joback Method

## Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R300702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R300702&amp;Units=SI</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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