

Tritriacontane, 5-methyl-

Other names:	5-Methyltritriacontane
Inchi:	InChI=1S/C34H70/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27
InchiKey:	FPKNBTAWMQVIW-UHFFFAOYSA-N
Formula:	C34H70
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]:	478.92

Physical Properties

Property code	Value	Unit	Source
gf	232.96	kJ/mol	Joback Method
hf	-750.37	kJ/mol	Joback Method
hfus	80.29	kJ/mol	Joback Method
hvap	90.89	kJ/mol	Joback Method
log10ws	-13.81		Crippen Method
logp	13.365		Crippen Method
mcvol	489.920	ml/mol	McGowan Method
pc	499.58	kPa	Joback Method
rinpol	3357.00		NIST Webbook
rinpol	3356.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook
rinpol	3344.00		NIST Webbook
tb	976.88	K	Joback Method
tc	1226.77	K	Joback Method
tf	457.94	K	Joback Method
vc	1.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.03	J/molxK	976.88	Joback Method
cpg	1787.83	J/molxK	1018.53	Joback Method
cpg	1817.45	J/molxK	1060.18	Joback Method

cpg	1845.07	J/molxK	1101.83	Joback Method
cpg	1870.84	J/molxK	1143.48	Joback Method
cpg	1894.95	J/molxK	1185.12	Joback Method
cpg	1917.55	J/molxK	1226.77	Joback Method
dvisc	0.0007325	Paxs	457.94	Joback Method
dvisc	0.0002138	Paxs	544.43	Joback Method
dvisc	0.0000875	Paxs	630.92	Joback Method
dvisc	0.0000444	Paxs	717.41	Joback Method
dvisc	0.0000261	Paxs	803.90	Joback Method
dvisc	0.0000170	Paxs	890.39	Joback Method
dvisc	0.0000119	Paxs	976.88	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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<https://www.chemeo.com/cid/50-091-5/Tritriacontane-5-methyl.pdf>

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