

13-Methyltritriacontane

Other names:	Tritriacontane, 13-methyl
Inchi:	InChI=1S/C34H70/c1-4-6-8-10-12-14-16-17-18-19-20-21-22-23-25-27-29-31-33-34(3)32
InchiKey:	TWDXTTZMADIJNW-UHFFFAOYSA-N
Formula:	C34H70
SMILES:	CCCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCC
Mol. weight [g/mol]:	478.92
CAS:	56987-76-9

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	3328.00		NIST Webbook
rinpol	3332.00		NIST Webbook
rinpol	3332.00		NIST Webbook
rinpol	3325.00		NIST Webbook
rinpol	3329.00		NIST Webbook
rinpol	3335.00		NIST Webbook
rinpol	3329.00		NIST Webbook
rinpol	3329.00		NIST Webbook
rinpol	3327.00		NIST Webbook
rinpol	3333.00		NIST Webbook
rinpol	3333.00		NIST Webbook
rinpol	3330.00		NIST Webbook
rinpol	3332.00		NIST Webbook
rinpol	3329.00		NIST Webbook
rinpol	3338.00		NIST Webbook
rinpol	3328.00		NIST Webbook
rinpol	3335.00		NIST Webbook
rinpol	3331.00		NIST Webbook
rinpol	3318.00		NIST Webbook

tb	976.88	K	Joback Method
tc	1226.77	K	Joback Method
tf	457.94	K	Joback Method
vc	1.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.03	J/mol×K	976.88	Joback Method
cpg	1894.95	J/mol×K	1185.12	Joback Method
cpg	1870.84	J/mol×K	1143.48	Joback Method
cpg	1845.07	J/mol×K	1101.83	Joback Method
cpg	1817.45	J/mol×K	1060.18	Joback Method
cpg	1787.83	J/mol×K	1018.53	Joback Method
cpg	1917.55	J/mol×K	1226.77	Joback Method
dvisc	0.0000119	Paxs	976.88	Joback Method
dvisc	0.0000170	Paxs	890.39	Joback Method
dvisc	0.0000261	Paxs	803.90	Joback Method
dvisc	0.0000444	Paxs	717.41	Joback Method
dvisc	0.0000875	Paxs	630.92	Joback Method
dvisc	0.0002138	Paxs	544.43	Joback Method
dvisc	0.0007325	Paxs	457.94	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56987769&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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>

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
hvac:	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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