

14,18,22,26-Tetramethyl-nonacosyl cyanide

Inchi:	InChI=1S/C34H67N/c1-6-22-31(2)24-19-26-33(4)28-21-29-34(5)27-20-25-32(3)23-17-15
InchiKey:	ISHPSUZCJIFPAT-UHFFFAOYSA-N
Formula:	C34H67N
SMILES:	CCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	489.90

Physical Properties

Property code	Value	Unit	Source
gf	358.82	kJ/mol	Joback Method
hf	-601.33	kJ/mol	Joback Method
hfus	71.23	kJ/mol	Joback Method
hvap	100.20	kJ/mol	Joback Method
log10ws	-12.95		Crippen Method
logp	12.437		Crippen Method
mcvol	491.300	ml/mol	McGowan Method
pc	499.36	kPa	Joback Method
rinsol	3482.00		NIST Webbook
tb	1077.64	K	Joback Method
tc	1360.28	K	Joback Method
tf	477.93	K	Joback Method
vc	1.942	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1805.17	J/molxK	1077.64	Joback Method
cpg	1834.01	J/molxK	1124.75	Joback Method
cpg	1860.61	J/molxK	1171.85	Joback Method
cpg	1885.19	J/molxK	1218.96	Joback Method
cpg	1908.00	J/molxK	1266.07	Joback Method
cpg	1929.27	J/molxK	1313.17	Joback Method
cpg	1949.26	J/molxK	1360.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202252&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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