16,20,24-Trimethyl-hentriacontyl cyanide

Inchi: InChI=1S/C35H69N/c1-5-6-7-18-21-26-33(2)28-24-30-35(4)31-25-29-34(3)27-22-19-16-1
InchiKey: VKVVQYUZIIXQDK-UHFFFAOYSA-N
Formula: C35H69N
SMILES: CCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 503.93

Physical Properties

Property code	Value	Unit	Source
gf	369.68	kJ/mol	Joback Method
hf	-616.69	kJ/mol	Joback Method
hfus	77.34	kJ/mol	Joback Method
hvap	102.82	kJ/mol	Joback Method
log10ws	-13.61		Crippen Method
logp	12.971		Crippen Method
mcvol	505.390	ml/mol	McGowan Method
pc	476.93	kPa	Joback Method
rinpol	3632.00		NIST Webbook
rinpol	3632.00		NIST Webbook
tb	1100.96	K	Joback Method
tc	1405.51	K	Joback Method
tf	504.20	K	Joback Method
vc	2.003	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1873.08	J/mol×K	1100.96	Joback Method
cpg	1903.90	J/mol×K	1151.72	Joback Method
cpg	1932.22	J/mol×K	1202.48	Joback Method
cpg	1958.35	J/mol×K	1253.23	Joback Method
cpg	1982.60	J/mol×K	1303.99	Joback Method
cpg	2005.29	J/mol×K	1354.75	Joback Method
cpg	2026.73	J/mol×K	1405.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202316&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume