20-Methyl-dotriacontyl cyanide

Inchi: InChI=1S/C34H67N/c1-3-4-5-6-7-8-19-22-25-28-31-34(2)32-29-26-23-20-17-15-13-11-9-

InchiKey: VGTYWFIKOFXUSE-UHFFFAOYSA-N

Formula: C34H67N

SMILES: CCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCCC#N

Mol. weight [g/mol]: 489.90

Physical Properties

Property code	Value	Unit	Source
gf	366.14	kJ/mol	Joback Method
hf	-585.49	kJ/mol	Joback Method
hfus	81.80	kJ/mol	Joback Method
hvap	101.37	kJ/mol	Joback Method
log10ws	-13.68		Crippen Method
logp	12.869		Crippen Method
mcvol	491.300	ml/mol	McGowan Method
pc	494.05	kPa	Joback Method
rinpol	3687.00		NIST Webbook
rinpol	3687.00		NIST Webbook
tb	1078.96	K	Joback Method
tc	1374.69	K	Joback Method
tf	522.93	K	Joback Method
vc	1.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1804.95	J/mol×K	1078.96	Joback Method
cpg	1835.45	J/mol×K	1128.25	Joback Method
cpg	1863.57	J/mol×K	1177.54	Joback Method
cpg	1889.59	J/mol×K	1226.83	Joback Method
cpg	1913.79	J/mol×K	1276.12	Joback Method
cpg	1936.44	J/mol×K	1325.41	Joback Method
cpg	1957.83	J/mol×K	1374.69	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=R202618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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