16,20-Dimethyl-hentriacontyl cyanide

Inchi: InChI=1S/C34H67N/c1-4-5-6-7-8-15-18-21-24-28-33(2)30-27-31-34(3)29-25-22-19-16-13
InchiKey: SBUSRZPUTHJFHZ-UHFFFAOYSA-N
Formula: C34H67N
SMILES: CCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 489.90

Physical Properties

Property code	Value	Unit	Source
gf	363.70	kJ/mol	Joback Method
hf	-590.77	kJ/mol	Joback Method
hfus	78.28	kJ/mol	Joback Method
hvap	100.98	kJ/mol	Joback Method
log10ws	-13.44		Crippen Method
logp	12.725		Crippen Method
mcvol	491.300	ml/mol	McGowan Method
pc	495.81	kPa	Joback Method
rinpol	3605.00		NIST Webbook
tb	1078.52	K	Joback Method
tc	1369.67	K	Joback Method
tf	507.93	K	Joback Method
vc	1.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1805.02	J/mol×K	1078.52	Joback Method
cpg	1834.94	J/mol×K	1127.05	Joback Method
cpg	1862.53	J/mol×K	1175.57	Joback Method
cpg	1888.05	J/mol×K	1224.10	Joback Method
cpg	1911.77	J/mol×K	1272.62	Joback Method
cpg	1933.94	J/mol×K	1321.15	Joback Method
cpg	1954.84	J/mol×K	1369.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202356&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume