18,22,26-Trimethyl-dotriacontyl cyanide

Inchi: InChI=1S/C36H71N/c1-5-6-7-22-27-34(2)29-25-31-36(4)32-26-30-35(3)28-23-20-18-16-1
InchiKey: HTBFLBWBWLBAKW-UHFFFAOYSA-N
Formula: C36H71N
SMILES: CCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 517.96

Physical Properties

Property code	Value	Unit	Source
gf	378.10	kJ/mol	Joback Method
hf	-637.33	kJ/mol	Joback Method
hfus	79.93	kJ/mol	Joback Method
hvap	105.04	kJ/mol	Joback Method
log10ws	-14.03		Crippen Method
logp	13.361		Crippen Method
mcvol	519.480	ml/mol	McGowan Method
pc	457.55	kPa	Joback Method
rinpol	3744.00		NIST Webbook
tb	1123.84	K	Joback Method
tc	1448.17	K	Joback Method
tf	515.47	K	Joback Method
vc	2.059	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1941.34	J/mol×K	1123.84	Joback Method
cpg	1973.76	J/mol×K	1177.89	Joback Method
cpg	2003.45	J/mol×K	1231.95	Joback Method
cpg	2030.81	J/mol×K	1286.00	Joback Method
cpg	2056.21	J/mol×K	1340.06	Joback Method
cpg	2080.05	J/mol×K	1394.11	Joback Method
cpg	2102.72	J/mol×K	1448.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202396&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