18,22-Dimethyl-triacontyl cyanide

Inchi: InChI=1S/C33H65N/c1-4-5-6-7-20-23-27-32(2)29-26-30-33(3)28-24-21-18-16-14-12-10-8
InchiKey: GJQUHEBKKWHVPC-UHFFFAOYSA-N
Formula: C33H65N
SMILES: CCCCCCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 475.88

Physical Properties

Property code	Value	Unit	Source
gf	355.28	kJ/mol	Joback Method
hf	-570.13	kJ/mol	Joback Method
hfus	75.69	kJ/mol	Joback Method
hvap	98.75	kJ/mol	Joback Method
log10ws	-13.02		Crippen Method
logp	12.335		Crippen Method
mcvol	477.210	ml/mol	McGowan Method
pc	517.70	kPa	Joback Method
rinpol	3509.00		NIST Webbook
rinpol	3509.00		NIST Webbook
tb	1055.64	K	Joback Method
tc	1330.28	K	Joback Method
tf	496.66	K	Joback Method
vc	1.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.27	J/mol×K	1055.64	Joback Method
cpg	1765.81	J/mol×K	1101.41	Joback Method
cpg	1792.22	J/mol×K	1147.19	Joback Method
cpg	1816.70	J/mol×K	1192.96	Joback Method
cpg	1839.47	J/mol×K	1238.73	Joback Method
cpg	1860.75	J/mol×K	1284.50	Joback Method
cpg	1880.75	J/mol×K	1330.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202490&Units=SI

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