22-Methyl-hentriacontyl cyanide

Inchi: InChI=1S/C33H65N/c1-3-4-5-6-21-24-27-30-33(2)31-28-25-22-19-17-15-13-11-9-7-8-10-
InchiKey: JRSFWTBPVPXVQS-UHFFFAOYSA-N
Formula: C33H65N
SMILES: CCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 475.88

Physical Properties

Property code	Value	Unit	Source
gf	357.72	kJ/mol	Joback Method
hf	-564.85	kJ/mol	Joback Method
hfus	79.21	kJ/mol	Joback Method
hvap	99.14	kJ/mol	Joback Method
log10ws	-13.26		Crippen Method
logp	12.479		Crippen Method
mcvol	477.210	ml/mol	McGowan Method
pc	515.83	kPa	Joback Method
rinpol	3589.00		NIST Webbook
rinpol	3589.00		NIST Webbook
tb	1056.08	K	Joback Method
tc	1334.66	K	Joback Method
tf	511.66	K	Joback Method
vc	1.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.14	J/mol×K	1056.08	Joback Method
cpg	1766.19	J/mol×K	1102.51	Joback Method
cpg	1793.05	J/mol×K	1148.94	Joback Method
cpg	1817.97	J/mol×K	1195.37	Joback Method
cpg	1841.16	J/mol×K	1241.80	Joback Method
cpg	1862.86	J/mol×K	1288.23	Joback Method
cpg	1883.28	J/mol×K	1334.66	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=R202698&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