18,22,26-Trimethyl-triacontyl cyanide

Inchi: InChI=1S/C34H67N/c1-5-6-25-32(2)27-23-29-34(4)30-24-28-33(3)26-21-19-17-15-13-11-
InchiKey: SDUWOTAOXBQQFV-UHFFFAOYSA-N
Formula: C34H67N
SMILES: CCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 489.90

Physical Properties

Property code	Value	Unit	Source
gf	361.26	kJ/mol	Joback Method
hf	-596.05	kJ/mol	Joback Method
hfus	74.75	kJ/mol	Joback Method
hvap	100.59	kJ/mol	Joback Method
log10ws	-13.20		Crippen Method
logp	12.581		Crippen Method
mcvol	491.300	ml/mol	McGowan Method
pc	497.58	kPa	Joback Method
rinpol	3549.00		NIST Webbook
rinpol	3549.00		NIST Webbook
tb	1078.08	K	Joback Method
tc	1364.87	K	Joback Method
tf	492.93	K	Joback Method
vc	1.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1805.09	J/mol×K	1078.08	Joback Method
cpg	1834.47	J/mol×K	1125.88	Joback Method
cpg	1861.55	J/mol×K	1173.68	Joback Method
cpg	1886.59	J/mol×K	1221.47	Joback Method
cpg	1909.84	J/mol×K	1269.27	Joback Method
cpg	1931.55	J/mol×K	1317.07	Joback Method
cpg	1951.98	J/mol×K	1364.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202430&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

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