18,22,26-Trimethyl-nonacosyl cyanide

Inchi: InChI=1S/C33H65N/c1-5-24-31(2)26-22-28-33(4)29-23-27-32(3)25-20-18-16-14-12-10-8-
InchiKey: XMTRGLQNTSHQKR-UHFFFAOYSA-N
Formula: C33H65N
SMILES: CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 475.88

Physical Properties

Property code	Value	Unit	Source
gf	352.84	kJ/mol	Joback Method
hf	-575.41	kJ/mol	Joback Method
hfus	72.16	kJ/mol	Joback Method
hvap	98.37	kJ/mol	Joback Method
log10ws	-12.78		Crippen Method
logp	12.191		Crippen Method
mcvol	477.210	ml/mol	McGowan Method
pc	519.59	kPa	Joback Method
rinpol	3466.00		NIST Webbook
rinpol	3466.00		NIST Webbook
tb	1055.20	K	Joback Method
tc	1326.09	K	Joback Method
tf	481.66	K	Joback Method
vc	1.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.40	J/mol×K	1055.20	Joback Method
cpg	1765.47	J/mol×K	1100.35	Joback Method
cpg	1791.43	J/mol×K	1145.50	Joback Method
cpg	1815.49	J/mol×K	1190.64	Joback Method
cpg	1837.86	J/mol×K	1235.79	Joback Method
cpg	1858.74	J/mol×K	1280.94	Joback Method
cpg	1878.34	J/mol×K	1326.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202410&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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