20,26-Dimethyl-nonacosyl cyanide

Inchi: InChI=1S/C32H63N/c1-4-26-31(2)27-23-21-24-29-32(3)28-22-19-17-15-13-11-9-7-5-6-8-

InchiKey: JUWQFCWTIRIVIR-UHFFFAOYSA-N

Formula: C32H63N

SMILES: CCCC(C)CCCCCC(C)CCCCCCCCCCCCCCCCCCCCCC#N

Mol. weight [g/mol]: 461.85

Physical Properties

Property code	Value	Unit	Source
gf	346.86	kJ/mol	Joback Method
hf	-549.49	kJ/mol	Joback Method
hfus	73.10	kJ/mol	Joback Method
hvap	96.53	kJ/mol	Joback Method
log10ws	-12.60		Crippen Method
logp	11.945		Crippen Method
mcvol	463.120	ml/mol	McGowan Method
pc	541.08	kPa	Joback Method
rinpol	3447.00		NIST Webbook
rinpol	3447.00		NIST Webbook
tb	1032.76	K	Joback Method
tc	1292.63	K	Joback Method
tf	485.39	K	Joback Method
vc	1.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1669.85	J/mol×K	1032.76	Joback Method
cpg	1697.14	J/mol×K	1076.07	Joback Method
cpg	1722.46	J/mol×K	1119.38	Joback Method
cpg	1746.01	J/mol×K	1162.70	Joback Method
cpg	1767.94	J/mol×K	1206.01	Joback Method
cpg	1788.44	J/mol×K	1249.32	Joback Method
cpg	1807.69	J/mol×K	1292.63	Joback Method

Sources

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=R202594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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