1,22,26-Trimethyl-octacosyl cyanide

Inchi: InChI=1S/C32H63N/c1-5-30(2)27-24-28-31(3)25-22-20-18-16-14-12-10-8-6-7-9-11-13-15
InchiKey: RUHUGRTZLUWFDB-UHFFFAOYSA-N
Formula: C32H63N
SMILES: CCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCCCCCC(C)C#N
Mol. weight [g/mol]: 461.85

Physical Properties

Property code	Value	Unit	Source
gf	344.42	kJ/mol	Joback Method
hf	-554.77	kJ/mol	Joback Method
hfus	69.57	kJ/mol	Joback Method
hvap	96.14	kJ/mol	Joback Method
log10ws	-12.36		Crippen Method
logp	11.801		Crippen Method
mcvol	463.120	ml/mol	McGowan Method
pc	543.10	kPa	Joback Method
rinpol	3389.00		NIST Webbook
tb	1032.32	K	Joback Method
tc	1289.02	K	Joback Method
tf	470.39	K	Joback Method
vc	1.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.03	J/mol×K	1032.32	Joback Method
cpg	1696.91	J/mol×K	1075.10	Joback Method
cpg	1721.86	J/mol×K	1117.89	Joback Method
cpg	1745.04	J/mol×K	1160.67	Joback Method
cpg	1766.62	J/mol×K	1203.46	Joback Method
cpg	1786.78	J/mol×K	1246.24	Joback Method
cpg	1805.69	J/mol×K	1289.02	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=R202232&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