18,22-Dimethyl-tetratriacontyl cyanide

Inchi: InChI=1S/C37H73N/c1-4-5-6-7-8-9-18-21-24-27-31-36(2)33-30-34-37(3)32-28-25-22-19-
InchiKey: SHUHFLPYJWDATQ-UHFFFAOYSA-N
Formula: C37H73N
SMILES: CCCCCCCCCCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 531.98

Physical Properties

Property code	Value	Unit	Source
gf	388.96	kJ/mol	Joback Method
hf	-652.69	kJ/mol	Joback Method
hfus	86.05	kJ/mol	Joback Method
hvap	107.66	kJ/mol	Joback Method
log10ws	-14.69		Crippen Method
logp	13.895		Crippen Method
mcvol	533.570	ml/mol	McGowan Method
pc	437.85	kPa	Joback Method
rinpol	3902.00		NIST Webbook
rinpol	3902.00		NIST Webbook
tb	1147.16	K	Joback Method
tc	1499.99	K	Joback Method
tf	541.74	K	Joback Method
vc	2.122	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2009.99	J/mol×K	1147.16	Joback Method
cpg	2044.98	J/mol×K	1205.97	Joback Method
cpg	2076.94	J/mol×K	1264.77	Joback Method
cpg	2106.38	J/mol×K	1323.58	Joback Method
cpg	2133.82	J/mol×K	1382.38	Joback Method
cpg	2159.77	J/mol×K	1441.19	Joback Method
cpg	2184.75	J/mol×K	1499.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202485&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

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