14,18,22,26-Tetramethyl-hentriacontyl cyanide

Inchi: InChI=1S/C36H71N/c1-6-7-18-24-33(2)26-21-28-35(4)30-23-31-36(5)29-22-27-34(3)25-1
InchiKey: MHQFPPBLKBJQCX-UHFFFAOYSA-N
Formula: C36H71N
SMILES: CCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 517.96

Physical Properties

Property code	Value	Unit	Source
gf	375.66	kJ/mol	Joback Method
hf	-642.61	kJ/mol	Joback Method
hfus	76.41	kJ/mol	Joback Method
hvap	104.66	kJ/mol	Joback Method
log10ws	-13.79		Crippen Method
logp	13.217		Crippen Method
mcvol	519.480	ml/mol	McGowan Method
pc	459.12	kPa	Joback Method
rinpol	3652.00		NIST Webbook
rinpol	3652.00		NIST Webbook
tb	1123.40	K	Joback Method
tc	1442.22	K	Joback Method
tf	500.47	K	Joback Method
vc	2.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1941.28	J/mol×K	1123.40	Joback Method
cpg	1973.02	J/mol×K	1176.54	Joback Method
cpg	2002.08	J/mol×K	1229.67	Joback Method
cpg	2028.84	J/mol×K	1282.81	Joback Method
cpg	2053.66	J/mol×K	1335.95	Joback Method
cpg	2076.92	J/mol×K	1389.08	Joback Method
cpg	2098.97	J/mol×K	1442.22	Joback Method

Sources

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=R202247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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