16,20,24,28-Tetramethyl-dotriacontyl cyanide

Inchi: InChI=1S/C38H75N/c1-6-7-20-26-35(2)28-23-30-37(4)32-25-33-38(5)31-24-29-36(3)27-2
InchiKey: BWXBVTOVNIYNMS-UHFFFAOYSA-N
Formula: C38H75N
SMILES: CCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 546.01

Physical Properties

Property code	Value	Unit	Source
gf	392.50	kJ/mol	Joback Method
hf	-683.89	kJ/mol	Joback Method
hfus	81.59	kJ/mol	Joback Method
hvap	109.11	kJ/mol	Joback Method
log10ws	-14.63		Crippen Method
logp	13.997		Crippen Method
mcvol	547.660	ml/mol	McGowan Method
pc	423.55	kPa	Joback Method
rinpol	3766.00		NIST Webbook
tb	1169.16	K	Joback Method
tc	1532.73	K	Joback Method
tf	523.01	K	Joback Method
vc	2.166	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2078.42	J/mol×K	1169.16	Joback Method
cpg	2113.68	J/mol×K	1229.75	Joback Method
cpg	2145.80	J/mol×K	1290.35	Joback Method
cpg	2175.34	J/mol×K	1350.94	Joback Method
cpg	2202.89	J/mol×K	1411.54	Joback Method
cpg	2229.03	J/mol×K	1472.13	Joback Method
cpg	2254.32	J/mol×K	1532.73	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=R202267&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