

18,22,26-Trimethyl-tetratriacontyl cyanide

Inchi:	InChI=1S/C38H75N/c1-5-6-7-8-21-24-29-36(2)31-27-33-38(4)34-28-32-37(3)30-25-22-19
InchiKey:	KBSJZGIEPKDNNM-UHFFFAOYSA-N
Formula:	C38H75N
SMILES:	CCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	546.01

Physical Properties

Property code	Value	Unit	Source
gf	394.94	kJ/mol	Joback Method
hf	-678.61	kJ/mol	Joback Method
hfus	85.11	kJ/mol	Joback Method
hvap	109.50	kJ/mol	Joback Method
log10ws	-14.87		Crippen Method
logp	14.141		Crippen Method
mvol	547.660	ml/mol	McGowan Method
pc	422.16	kPa	Joback Method
rinpol	3926.00		NIST Webbook
tb	1169.60	K	Joback Method
tc	1540.26	K	Joback Method
tf	538.01	K	Joback Method
vc	2.171	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2078.62	J/molxK	1169.60	Joback Method
cpg	2114.76	J/molxK	1231.38	Joback Method
cpg	2147.68	J/molxK	1293.15	Joback Method
cpg	2177.99	J/molxK	1354.93	Joback Method
cpg	2206.31	J/molxK	1416.71	Joback Method
cpg	2233.25	J/molxK	1478.49	Joback Method
cpg	2259.42	J/molxK	1540.26	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=R202425&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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