

16,20,24-Trimethyl-tetratriacontyl cyanide

Inchi: InChI=1S/C39H77N/c1-5-6-7-8-9-16-19-22-25-30-37(2)32-28-34-39(4)35-29-33-38(3)31-
InchiKey: OUMPAWHKSURNBE-UHFFFAOYSA-N
Formula: C39H77N
SMILES: CCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 560.04

Physical Properties

Property code	Value	Unit	Source
gf	403.36	kJ/mol	Joback Method
hf	-699.25	kJ/mol	Joback Method
hfus	87.70	kJ/mol	Joback Method
hvap	111.72	kJ/mol	Joback Method
log10ws	-15.29		Crippen Method
logp	14.531		Crippen Method
mvol	561.750	ml/mol	McGowan Method
pc	405.99	kPa	Joback Method
rinpol	3923.00		NIST Webbook
tb	1192.48	K	Joback Method
tc	1590.12	K	Joback Method
tf	549.28	K	Joback Method
vc	2.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2147.62	J/mol×K	1192.48	Joback Method
cpg	2185.92	J/mol×K	1258.75	Joback Method
cpg	2220.75	J/mol×K	1325.03	Joback Method
cpg	2252.87	J/mol×K	1391.30	Joback Method
cpg	2283.08	J/mol×K	1457.57	Joback Method
cpg	2312.15	J/mol×K	1523.84	Joback Method
cpg	2340.85	J/mol×K	1590.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202321&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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