22,26-Dimethyl-dotriacontyl cyanide

Inchi: InChI=1S/C35H69N/c1-4-5-6-25-29-34(2)31-28-32-35(3)30-26-23-21-19-17-15-13-11-9-7

InchiKey: OFGLMZDVZPZSIL-UHFFFAOYSA-N

Formula: C35H69N

SMILES: CCCCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCCCCCC#N

Mol. weight [g/mol]: 503.93

Physical Properties

Property code	Value	Unit	Source
gf	372.12	kJ/mol	Joback Method
hf	-611.41	kJ/mol	Joback Method
hfus	80.87	kJ/mol	Joback Method
hvap	103.21	kJ/mol	Joback Method
log10ws	-13.86		Crippen Method
logp	13.115		Crippen Method
mcvol	505.390	ml/mol	McGowan Method
pc	475.27	kPa	Joback Method
rinpol	3715.00		NIST Webbook
rinpol	3715.00		NIST Webbook
tb	1101.40	K	Joback Method
tc	1410.98	K	Joback Method
tf	519.20	K	Joback Method
vc	2.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1873.07	J/mol×K	1101.40	Joback Method
cpg	1904.52	J/mol×K	1153.00	Joback Method
cpg	1933.42	J/mol×K	1204.59	Joback Method
cpg	1960.10	J/mol×K	1256.19	Joback Method
cpg	1984.88	J/mol×K	1307.79	Joback Method
cpg	2008.10	J/mol×K	1359.38	Joback Method
cpg	2030.08	J/mol×K	1410.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202643&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
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
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

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