22,26-Dimethyl-tritriacontyl cyanide

Inchi: InChI=1S/C36H71N/c1-4-5-6-23-26-30-35(2)32-29-33-36(3)31-27-24-21-19-17-15-13-11-
InchiKey: RQZNUFNZGDUOPX-UHFFFAOYSA-N
Formula: C36H71N
SMILES: CCCCCCCC(C)CCCC(C)CCCCCCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 517.96

Physical Properties

Property code	Value	Unit	Source
gf	380.54	kJ/mol	Joback Method
hf	-632.05	kJ/mol	Joback Method
hfus	83.46	kJ/mol	Joback Method
hvap	105.43	kJ/mol	Joback Method
log10ws	-14.28		Crippen Method
logp	13.505		Crippen Method
mcvol	519.480	ml/mol	McGowan Method
pc	455.99	kPa	Joback Method
rinpol	3814.00		NIST Webbook
rinpol	3814.00		NIST Webbook
tb	1124.28	K	Joback Method
tc	1454.36	K	Joback Method
tf	530.47	K	Joback Method
vc	2.066	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1941.40	J/mol×K	1124.28	Joback Method
cpg	1974.53	J/mol×K	1179.29	Joback Method
cpg	2004.88	J/mol×K	1234.31	Joback Method
cpg	2032.86	J/mol×K	1289.32	Joback Method
cpg	2058.87	J/mol×K	1344.33	Joback Method
cpg	2083.33	J/mol×K	1399.35	Joback Method
cpg	2106.64	J/mol×K	1454.36	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=R202678&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