28-Methyl-triacontyl cyanide

Inchi: InChI=1S/C32H63N/c1-3-32(2)30-28-26-24-22-20-18-16-14-12-10-8-6-4-5-7-9-11-13-15-
InchiKey: DABXOZVINIJWEL-UHFFFAOYSA-N
Formula: C32H63N
SMILES: CCC(C)CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 461.85

Physical Properties

Property code	Value	Unit	Source
gf	349.30	kJ/mol	Joback Method
hf	-544.21	kJ/mol	Joback Method
hfus	76.62	kJ/mol	Joback Method
hvap	96.92	kJ/mol	Joback Method
log10ws	-12.84		Crippen Method
logp	12.089		Crippen Method
mcvol	463.120	ml/mol	McGowan Method
pc	539.08	kPa	Joback Method
rinpol	3531.00		NIST Webbook
rinpol	3531.00		NIST Webbook
tb	1033.20	K	Joback Method
tc	1296.44	K	Joback Method
tf	500.39	K	Joback Method
vc	1.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1669.67	J/mol×K	1033.20	Joback Method
cpg	1697.39	J/mol×K	1077.07	Joback Method
cpg	1723.11	J/mol×K	1120.95	Joback Method
cpg	1747.03	J/mol×K	1164.82	Joback Method
cpg	1769.33	J/mol×K	1208.69	Joback Method
cpg	1790.19	J/mol×K	1252.56	Joback Method
cpg	1809.80	J/mol×K	1296.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R202732&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