

22-Methyl-tritriacontyl cyanide

Inchi: InChI=1S/C35H69N/c1-3-4-5-6-7-20-23-26-29-32-35(2)33-30-27-24-21-18-16-14-12-10-8
InchiKey: UYEHKWKWOSPIIC-UHFFFAOYSA-N
Formula: C35H69N
SMILES: CCCCCCCCCCCC(C)CCCCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 503.93

Physical Properties

Property code	Value	Unit	Source
gf	374.56	kJ/mol	Joback Method
hf	-606.13	kJ/mol	Joback Method
hfus	84.39	kJ/mol	Joback Method
hvap	103.59	kJ/mol	Joback Method
log10ws	-14.10		Crippen Method
logp	13.259		Crippen Method
mcvol	505.390	ml/mol	McGowan Method
pc	473.62	kPa	Joback Method
rinpol	3785.00		NIST Webbook
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tb	1101.84	K	Joback Method
tc	1416.68	K	Joback Method
tf	534.20	K	Joback Method
vc	2.015	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1873.06	J/molxK	1101.84	Joback Method
cpg	1905.17	J/molxK	1154.31	Joback Method
cpg	1934.67	J/molxK	1206.79	Joback Method
cpg	1961.92	J/molxK	1259.26	Joback Method
cpg	1987.26	J/molxK	1311.74	Joback Method
cpg	2011.03	J/molxK	1364.21	Joback Method
cpg	2033.59	J/molxK	1416.68	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=R202712&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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