26-Methyl-octacosyl cyanide

Inchi: InChI=1S/C30H59N/c1-3-30(2)28-26-24-22-20-18-16-14-12-10-8-6-4-5-7-9-11-13-15-17-
InchiKey: SNYRMAGWMGAKRY-UHFFFAOYSA-N
Formula: C30H59N
SMILES: CCC(C)CCCCCCCCCCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]: 433.80

Physical Properties

Property code	Value	Unit	Source
gf	332.46	kJ/mol	Joback Method
hf	-502.93	kJ/mol	Joback Method
hfus	71.44	kJ/mol	Joback Method
hvap	92.46	kJ/mol	Joback Method
log10ws	-12.01		Crippen Method
logp	11.309		Crippen Method
mcvol	434.940	ml/mol	McGowan Method
pc	590.55	kPa	Joback Method
rinpol	3329.00		NIST Webbook
tb	987.44	K	Joback Method
tc	1224.84	K	Joback Method
tf	477.85	K	Joback Method
vc	1.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1535.81	J/mol×K	987.44	Joback Method
cpg	1561.25	J/mol×K	1027.01	Joback Method
cpg	1585.00	J/mol×K	1066.57	Joback Method
cpg	1607.20	J/mol×K	1106.14	Joback Method
cpg	1627.98	J/mol×K	1145.71	Joback Method
cpg	1647.46	J/mol×K	1185.28	Joback Method
cpg	1665.76	J/mol×K	1224.84	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=R202727&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

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