2,4,6-tris-Cyano-1-hexene

Inchi: InChI=1S/C9H9N3/c1-8(6-11)5-9(7-12)3-2-4-10/h9H,1-3,5H2
InchiKey: RCOYANLEFOLXNT-UHFFFAOYSA-N
Formula: C9H9N3
SMILES: C=C(C#N)CC(C#N)CCC#N
Mol. weight [g/mol]: 159.19

Physical Properties

Property code	Value	Unit	Source
gf	501.29	kJ/mol	Joback Method
hf	375.91	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	66.08	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.900		Crippen Method
mcvol	137.510	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1520.00		NIST Webbook
tb	707.68	K	Joback Method
tc	930.73	K	Joback Method
tf	355.44	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.62	J/mol×K	707.68	Joback Method
cpg	341.71	J/mol×K	744.85	Joback Method
cpg	349.29	J/mol×K	782.03	Joback Method
cpg	356.38	J/mol×K	819.20	Joback Method
cpg	363.00	J/mol×K	856.38	Joback Method
cpg	369.20	J/mol×K	893.55	Joback Method
cpg	375.00	J/mol×K	930.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582162&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