2,4-Hexadienenitrile

Inchi: InChI=1S/C6H7N/c1-2-3-4-5-6-7/h2-5H,1H3/b3-2+,5-4+
InchiKey: NYKHMTWWXWMMHN-MQQKCMAXSA-N
Formula: C6H7N
SMILES: CC=CC=CC#N
Mol. weight [g/mol]: 93.13
CAS: 1516-01-4

Physical Properties

Property code	Value	Unit	Source
gf	293.26	kJ/mol	Joback Method
hf	232.15	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	39.34	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.642		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	447.08	K	Joback Method
tc	655.57	K	Joback Method
tf	212.21	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.85	J/mol×K	447.08	Joback Method
cpg	165.08	J/mol×K	481.83	Joback Method
cpg	172.77	J/mol×K	516.58	Joback Method
cpg	179.96	J/mol×K	551.33	Joback Method
cpg	186.68	J/mol×K	586.07	Joback Method
cpg	192.97	J/mol×K	620.82	Joback Method
cpg	198.87	J/mol×K	655.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.50 ± 0.50	K	2.10	NIST Webbook

Sources

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=C1516014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume