Hexanenitrile, 5-methyl-

Other names:	5-Methylhexanenitrile
	4-Methylpentyl cyanide
Inchi:	InChI=1S/C7H13N/c1-7(2)5-3-4-6-8/h7H,3-5H2,1-2H3
InchiKey:	CHWIKAJVZUSSML-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	CC(C)CCCC#N
Mol. weight [g/mol]:	111.18
CAS:	19424-34-1

Physical Properties

Property code	Value	Unit	Source
gf	138.80	kJ/mol	Joback Method
hf	-28.21	kJ/mol	Joback Method
hfus	11.87	kJ/mol	Joback Method
hvap	41.27	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.336		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	928.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	942.10		NIST Webbook
rinpol	910.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1350.00		NIST Webbook
ripol	1337.00		NIST Webbook
tb	461.20	K	Joback Method
tc	652.47	K	Joback Method
tf	218.64	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.35	J/mol×K	461.20	Joback Method
cpg	240.19	J/mol×K	493.08	Joback Method
cpg	250.55	J/mol×K	524.96	Joback Method
cpg	260.46	J/mol×K	556.84	Joback Method
cpg	269.92	J/mol×K	588.72	Joback Method
cpg	278.94	J/mol×K	620.60	Joback Method
cpg	287.54	J/mol×K	652.47	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19424341&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume