Pentanenitrile, 5-(methylthio)-

Other names:	4-(Methylthio)butyl cyanide
	5-Methylthiopentanonitrile
	5-Methylthiopentyl nitrile
	5-(Methylthio)pentanenitrile
Inchi:	InChI=1S/C6H11NS/c1-8-6-4-2-3-5-7/h2-4,6H2,1H3
InchiKey:	XPUDGEZWSNPCMM-UHFFFAOYSA-N
Formula:	C6H11NS
SMILES:	CSCCCCC#N
Mol. weight [g/mol]:	129.22
CAS:	59121-25-4

Physical Properties

Property code	Value	Unit	Source
gf	165.94	kJ/mol	Joback Method
hf	39.58	kJ/mol	Joback Method
hfus	16.93	kJ/mol	Joback Method
hvap	46.25	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	2.043		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1202.30		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1211.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1850.00		NIST Webbook
tb	507.54	K	Joback Method
tc	717.83	K	Joback Method
tf	256.77	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.16	J/mol×K	507.54	Joback Method
cpg	243.04	J/mol×K	542.59	Joback Method
cpg	252.45	J/mol×K	577.64	Joback Method
cpg	261.41	J/mol×K	612.69	Joback Method
cpg	269.91	J/mol×K	647.73	Joback Method
cpg	277.98	J/mol×K	682.78	Joback Method
cpg	285.60	J/mol×K	717.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59121254&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

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