

Butanenitrile, 4-(methylthio)-

Other names:3-(Methylthio)propyl cyanide
4-Methylthio butanenitrile
4-Methylthiobutyl nitrile

Inchi:InChI=1S/C5H9NS/c1-7-5-3-2-4-6/h2-3,5H2,1H3

InchiKey:JPWPMBYFDCHLKL-UHFFFAOYSA-N

Formula:C5H9NS

SMILES:CSCCCC#N

Mol. weight [g/mol]:115.20

CAS:59121-24-3

Physical Properties

Property code	Value	Unit	Source
gf	157.52	kJ/mol	Joback Method
hf	60.22	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	44.02	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.653		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1051.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1806.00		NIST Webbook
tb	484.66	K	Joback Method
tc	698.19	K	Joback Method
tf	245.50	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.75	J/mol×K	484.66	Joback Method
cpg	201.33	J/mol×K	520.25	Joback Method
cpg	209.52	J/mol×K	555.84	Joback Method
cpg	217.32	J/mol×K	591.43	Joback Method
cpg	224.73	J/mol×K	627.01	Joback Method
cpg	231.77	J/mol×K	662.60	Joback Method
cpg	238.43	J/mol×K	698.19	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=C59121243&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
mccvol:	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

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