

(Methylthio)-acetonitrile

Other names:	Acetonitrile, (methylthio)- CH ₃ SCH ₂ CN
Inchi:	InChI=1S/C3H5NS/c1-5-3-2-4/h3H2,1H3
InchiKey:	ZRIGDBVSVFVLL-UHFFFAOYSA-N
Formula:	C ₃ H ₅ NS
SMILES:	CSCC#N
Mol. weight [g/mol]:	87.14
CAS:	35120-10-6

Physical Properties

Property code	Value	Unit	Source
affp	784.80	kJ/mol	NIST Webbook
basg	754.10	kJ/mol	NIST Webbook
gf	140.68	kJ/mol	Joback Method
hf	101.50	kJ/mol	Joback Method
hfus	9.16	kJ/mol	Joback Method
hvap	39.57	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.873		Crippen Method
mvol	70.860	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	438.90	K	Joback Method
tc	658.75	K	Joback Method
tf	222.96	K	Joback Method
vc	0.283	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.51	J/mol×K	438.90	Joback Method
cpg	124.00	J/mol×K	475.54	Joback Method
cpg	129.27	J/mol×K	512.18	Joback Method
cpg	134.31	J/mol×K	548.82	Joback Method
cpg	139.14	J/mol×K	585.47	Joback Method

cpg	143.73	J/mol×K	622.11	Joback Method
cpg	148.09	J/mol×K	658.75	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	2.00	NIST Webbook

Sources

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=C35120106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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