methylthioacetaldehyde

Other names:	2-[Methylthio]ethanal
	2-Methylthioacetaldehyde
Inchi:	InChI=1S/C3H6OS/c1-5-3-2-4/h2H,3H2,1H3
InchiKey:	NCNSBFDGXBKAKB-UHFFFAOYSA-N
Formula:	C3H6OS
SMILES:	CSCC=O
Mol. weight [g/mol]:	90.14
CAS:	23328-62-3

Physical Properties

Property code	Value	Unit	Source
gf	-92.02	kJ/mol	Joback Method
hf	-148.96	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	35.81	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.548		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
ripol	1250.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1293.00		NIST Webbook
ripol	1270.00		NIST Webbook
ripol	1250.00		NIST Webbook
tb	385.48	K	Joback Method
tc	586.69	K	Joback Method
tf	199.97	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.50	J/mol×K	385.48	Joback Method

cpg	122.57	J/mol×K	419.01	Joback Method
cpg	128.42	J/mol×K	452.55	Joback Method
cpg	134.05	J/mol×K	486.08	Joback Method
cpg	139.45	J/mol×K	519.62	Joback Method
cpg	144.62	J/mol×K	553.15	Joback Method
cpg	149.57	J/mol×K	586.69	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=C23328623&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/91-629-3/methylthioacetaldehyde.pdf
Generated by Cheméo on 2024-10-12 05:50:20.882461884 +0000 UTC m=+3293083.519431133.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.