N-(methyl)mercaptoacetamide

Inchi: InChI=1S/C3H7NOS/c1-4-3(5)2-6/h6H,2H2,1H3,(H,4,5)
InchiKey: NSJNRJYQQPRCLF-UHFFFAOYSA-N
Formula: C3H7NOS
SMILES: CNC(=O)CS
Mol. weight [g/mol]: 105.16
CAS: 20938-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-35.76	kJ/mol	Joback Method
hf	-125.88	kJ/mol	Joback Method
hfus	14.27	kJ/mol	Joback Method
hvap	42.19	kJ/mol	Joback Method
log10ws	-0.12		Crippen Method
logp	-0.338		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	5359.18	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	938.00		NIST Webbook
tb	434.94	K	Joback Method
tc	646.04	K	Joback Method
tf	262.62	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.99	J/mol×K	434.94	Joback Method
cpg	153.39	J/mol×K	470.12	Joback Method
cpg	160.42	J/mol×K	505.31	Joback Method
cpg	167.09	J/mol×K	540.49	Joback Method
cpg	173.42	J/mol×K	575.67	Joback Method
cpg	179.41	J/mol×K	610.86	Joback Method
cpg	185.07	J/mol×K	646.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20938743&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume