Mercaptoacetone

Other names:	1-Sulfanylacetone
	1-Mercapto-2-propanone
	Mercapto-2-propanone
	2-Propanone, 1-mercapto-
	3-Mercapto-2-propanone
	mercaptopropanone
Inchi:	InChI=1S/C3H6OS/c1-3(4)2-5/h5H,2H2,1H3
InchiKey:	USVCRBGYQRVTNK-UHFFFAOYSA-N
Formula:	C3H6OS
SMILES:	CC(=O)CS
Mol. weight [g/mol]:	90.14
CAS:	24653-75-6

Physical Properties

Property code	Value	Unit	Source
gf	-125.15	kJ/mol	Joback Method
hf	-179.35	kJ/mol	Joback Method
hfus	9.17	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.505		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
rinpol	739.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	743.00		NIST Webbook
ripol	1357.00		NIST Webbook
ripol	1351.00		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1357.00		NIST Webbook
tb	384.77	K	Joback Method
tc	591.94	K	Joback Method
tf	209.96	K	Joback Method
vc	0.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.28	J/mol×K	384.77	Joback Method
cpg	119.61	J/mol×K	419.30	Joback Method
cpg	125.66	J/mol×K	453.83	Joback Method
cpg	131.44	J/mol×K	488.35	Joback Method
cpg	136.95	J/mol×K	522.88	Joback Method
cpg	142.20	J/mol×K	557.41	Joback Method
cpg	147.19	J/mol×K	591.94	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24653756&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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