

THIOACETIC S-ACID

Other names:	Methanecarbothiolic acid
	Thioacetic S-acid
	Ethanethioic acid
	Acetyl mercaptan
	Ethanethiolic acid
	Thiacetic acid
	Thiolacetic acid
	Thionoacetic acid
	CH3COSH
	Kyselina thiooctova
	UN 2436
	USAF EK-P-737
	Acetic acid, thio-
Inchi:	InChI=1S/C2H4OS/c1-2(3)4/h1H3,(H,3,4)
InchiKey:	DUYAAUVXQSMXQP-UHFFFAOYSA-N
Formula:	C2H4OS
SMILES:	CC(=O)S
Mol. weight [g/mol]:	76.12

Physical Properties

Property code	Value	Unit	Source
af	0.3447		Cheméo Relay (1.0)
chl	-1741.50	kJ/mol	NIST Webbook
gf	-133.57	kJ/mol	Joback Method
hf	-166.63	kJ/mol	Cheméo Relay (1.0)
hfl	-219.30 ± 1.50	kJ/mol	NIST Webbook
hfl	-216.50 ± 0.59	kJ/mol	NIST Webbook
hfus	6.58	kJ/mol	Joback Method
hvap	36.35	kJ/mol	Cheméo Relay (1.0)
ie	10.06	eV	NIST Webbook
log10ws	-0.05		Cheméo Relay (1.0)
logp	0.463		Crippen Method
mcvol	56.960	ml/mol	McGowan Method
pc	6075.01	kPa	Joback Method
ripol	1124.00		NIST Webbook
ripol	1124.00		NIST Webbook
tb	360.33	K	Cheméo Relay (1.0)

tc	581.01	K	Cheméo Relay (1.0)
tf	227.21	K	Cheméo Relay (1.0)
vc	0.192	m ³ /kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	82.03	J/mol×K	361.89	Joback Method
cpg	86.54	J/mol×K	396.68	Joback Method
cpg	90.87	J/mol×K	431.46	Joback Method
cpg	95.01	J/mol×K	466.25	Joback Method
cpg	98.96	J/mol×K	501.03	Joback Method
cpg	102.74	J/mol×K	535.82	Joback Method
cpg	106.34	J/mol×K	570.61	Joback Method
hvapt	35.20	kJ/mol	333.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507095&Units=SI

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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