

ACETIC ACID, (METHYLTHIO)-

Other names:	Acetic acid, (methylthio)- (methylthio)acetic acid
Inchi:	InChI=1S/C3H6O2S/c1-6-2-3(4)5/h2H2,1H3,(H,4,5)
InchiKey:	HGTBAIVLETUVCG-UHFFFAOYSA-N
Formula:	C3H6O2S
SMILES:	CSCC(=O)O
Mol. weight [g/mol]:	106.15

Physical Properties

Property code	Value	Unit	Source
af	0.5993		Cheméo Relay (1.0)
gf	-258.24	kJ/mol	Joback Method
hf	-424.51	kJ/mol	Cheméo Relay (1.0)
hfus	13.34	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Cheméo Relay (1.0)
ie	8.98	eV	Cheméo Relay (1.0)
logp	0.434		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	5619.38	kPa	Joback Method
tb	492.64	K	Cheméo Relay (1.0)
tc	712.92	K	Cheméo Relay (1.0)
tf	318.47	K	Cheméo Relay (1.0)
vc	0.253	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.94	J/mol×K	482.87	Joback Method
cpg	151.73	J/mol×K	515.60	Joback Method
cpg	157.27	J/mol×K	548.34	Joback Method
cpg	162.56	J/mol×K	581.07	Joback Method
cpg	167.61	J/mol×K	613.81	Joback Method
cpg	172.41	J/mol×K	646.54	Joback Method
cpg	176.96	J/mol×K	679.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.70	K	3.60	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2444373&Units=SI>

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):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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