

Acetic acid, mercapto-, ethyl ester

Other names:	Ethyl «alpha»-mercaptoacetate Ethyl mercaptoacetate Ethyl thioglycolate Ethyl thioglycollate Ethyl 2-mercaptoacetate Thioglycolic acid ethyl ester USAF EK-2070 Mercaptoacetic acid ethyl ester Thioglykolsaeure-aethylester Acetic acid, 2-mercapto-, ethyl ester NSC 8834
Inchi:	InChI=1S/C4H8O2S/c1-2-6-4(5)3-7/h7H,2-3H2,1H3
InchiKey:	PVBRSNZAOAJRKO-UHFFFAOYSA-N
Formula:	C4H8O2S
SMILES:	CCOC(=O)CS
Mol. weight [g/mol]:	120.17
CAS:	623-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-221.73	kJ/mol	Joback Method
hf	-332.21	kJ/mol	Joback Method
hfus	12.94	kJ/mol	Joback Method
hvap	40.39	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.479		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	430.20	K	NIST Webbook
tc	634.41	K	Joback Method
tf	243.46	K	Joback Method
vc	0.338	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.85	J/mol×K	430.07	Joback Method
cpg	174.67	J/mol×K	464.13	Joback Method
cpg	182.21	J/mol×K	498.18	Joback Method
cpg	189.48	J/mol×K	532.24	Joback Method
cpg	196.47	J/mol×K	566.30	Joback Method
cpg	203.17	J/mol×K	600.36	Joback Method
cpg	209.57	J/mol×K	634.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.20	K	1.60	NIST Webbook
tbrp	328.20	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
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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