Methyl 2-(methylthio)acetate

Other names:	Methyl (methylithio)acetate
	Acetic acid, (methylthio)-, methyl ester
	Methyl methylthioacetate
Inchi:	InChI=1S/C4H8O2S/c1-6-4(5)3-7-2/h3H2,1-2H3
InchiKey:	HZYCAKGEXXKCDM-UHFFFAOYSA-N
Formula:	C4H8O2S
SMILES:	COC(=O)CSC
Mol. weight [g/mol]:	120.17
CAS:	16630-66-3

Physical Properties

Property code	Value	Unit	Source
gf	-218.00	kJ/mol	Joback Method
hf	-328.82	kJ/mol	Joback Method
hfus	13.03	kJ/mol	Joback Method
hvap	40.47	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.522		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
rinpol	918.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	435.99	K	Joback Method
tc	640.35	K	Joback Method
tf	241.40	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.75	J/mol×K	435.99	Joback Method

cpg	175.63	J/mol×K	470.05	Joback Method
cpg	183.28	J/mol×K	504.11	Joback Method
cpg	190.68	J/mol×K	538.17	Joback Method
cpg	197.82	J/mol×K	572.23	Joback Method
cpg	204.68	J/mol×K	606.29	Joback Method
cpg	211.26	J/mol×K	640.35	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16630663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/96-682-9/Methyl-2-methylthio-acetate.pdf
Generated by Cheméo on 2024-04-29 07:38:17.278379164 +0000 UTC m=+16665546.198956477.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.