S-Methyl propanethioate

Other names:	S-Methyl thiopropanoate
	S-Methyl thiopropionate
	S-Methyl methylthiopropionate
Inchi:	InChI=1S/C4H8OS/c1-3-4(5)6-2/h3H2,1-2H3
InchiKey:	AIILTVHCLAEMDA-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	CCC(=O)SC
Mol. weight [g/mol]:	104.17
CAS:	5925-75-7

Physical Properties

Property code	Value	Unit	Source
gf	-113.00	kJ/mol	Joback Method
hf	-196.60	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	38.06	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.286		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1131.00		NIST Webbook
ripol	1130.00		NIST Webbook
ripol	1131.00		NIST Webbook
tb	413.57	K	Joback Method
tc	618.94	K	Joback Method
tf	219.17	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.97	J/mol×K	413.57	Joback Method
cpg	155.97	J/mol×K	447.80	Joback Method
cpg	163.66	J/mol×K	482.03	Joback Method
cpg	171.03	J/mol×K	516.25	Joback Method
cpg	178.09	J/mol×K	550.48	Joback Method
cpg	184.83	J/mol×K	584.71	Joback Method
cpg	191.25	J/mol×K	618.94	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=C5925757&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