Cyclopentane, (methylthio)-

Other names:	Sulfide, cyclopentyl methyl
	Cyclopentyl methyl sulfide
	Methyl cyclopentyl sulfide
	Methylthiocyclopentane
	Cyclopentyl methyl sulphide
	(Methylsulfanyl)cyclopentane
	Cyclopentyl-1-thiaethane
Inchi:	InChI=1S/C6H12S/c1-7-6-4-2-3-5-6/h6H,2-5H2,1H3
InchiKey:	OTQVGYMGQKHLMY-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	CSC1CCCC1
Mol. weight [g/mol]:	116.22
CAS:	7133-36-0

Physical Properties

Property code	Value	Unit	Source
chl	-4568.26 ± 0.84	kJ/mol	NIST Webbook
gf	69.31	kJ/mol	Joback Method
hf	-64.35 ± 0.96	kJ/mol	NIST Webbook
hfl	-109.50 ± 0.92	kJ/mol	NIST Webbook
hfus	9.36	kJ/mol	Joback Method
hvap	45.10 ± 0.10	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
hvap	45.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.22		Crippen Method
logp	2.292		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
sl	285.47	J/mol×K	NIST Webbook
tb	431.70	K	NIST Webbook
tc	643.98	K	Joback Method
tf	202.68	K	Joback Method
tt	169.86 ± 0.06	K	NIST Webbook
tt	169.85 ± 0.04	K	NIST Webbook

tt	169.34 ± 0.04	K	NIST Webbook
tt	169.86 ± 0.06	K	NIST Webbook
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.25	J/mol×K	457.95	Joback Method
cpg	264.88	J/mol×K	643.98	Joback Method
cpg	253.83	J/mol×K	606.77	Joback Method
cpg	242.06	J/mol×K	569.56	Joback Method
cpg	229.56	J/mol×K	532.36	Joback Method
cpg	216.30	J/mol×K	495.15	Joback Method
cpg	187.40	J/mol×K	420.74	Joback Method
cpl	192.92	J/mol×K	298.15	NIST Webbook
hfust	9.20	kJ/mol	169.90	NIST Webbook
hfust	0.90	kJ/mol	165.00	NIST Webbook
hfust	9.20	kJ/mol	169.90	NIST Webbook
hvapt	41.70	kJ/mol	413.50	NIST Webbook
sfust	54.31	J/mol×K	169.90	NIST Webbook
sfust	5.44	J/mol×K	165.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7133360&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume