Propane, 2-methyl-1-(methylthio)-

Other names:	4-Methyl-2-thiapentane
	Isobutyl methyl sulfide
	Methyl isobutyl sulfide
	Sulfide, isobutyl methyl
Inchi:	InChI=1S/C5H12S/c1-5(2)4-6-3/h5H,4H2,1-3H3
InchiKey:	UYVGFIKOUAFDOZ-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CSCC(C)C
Mol. weight [g/mol]:	104.21
CAS:	5008-69-5

Physical Properties

Property code	Value	Unit	Source
gf	21.90	kJ/mol	Joback Method
hf	-109.94	kJ/mol	Joback Method
hfus	9.31	kJ/mol	Joback Method
hvap	33.15	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	2.005		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	775.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	763.00		NIST Webbook
tb	386.25 ± 0.30	K	NIST Webbook
tc	576.94	K	Joback Method
tf	164.05 ± 0.20	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.80	J/mol×K	544.47	Joback Method
cpg	169.65	J/mol×K	382.14	Joback Method
cpg	180.05	J/mol×K	414.61	Joback Method
cpg	190.07	J/mol×K	447.07	Joback Method
cpg	199.69	J/mol×K	479.54	Joback Method
cpg	208.93	J/mol×K	512.01	Joback Method
cpg	226.28	J/mol×K	576.94	Joback Method
hvapt	36.90	kJ/mol	349.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37307e+01
Coeff. B	-2.92807e+03
Coeff. C	-6.49210e+01
Temperature range (K), min.	282.73
Temperature range (K), max.	412.70

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5008695&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume