1-Propanol, 3-(methylthio)-

Other names:	«gamma»-Methylmercaptopropyl alcohol
	3-(Methylthio)-1-propanol
	3-Hydroxypropyl methyl sulfide
	3-Methylmercapto-1-propanol
	3-(Methylthio)propanol
	3-(Methylsulfanyl)propanol
	3-Methylthiopropyl alcohol
	Methionol
	NSC 2859
	3-(methylsulfanyl)propanol (methionol)
Inchi:	InChI=1S/C4H10OS/c1-6-4-2-3-5/h5H,2-4H2,1H3
InchiKey:	CZUGFKJYCPYHHV-UHFFFAOYSA-N
Formula:	C4H10OS
SMILES:	CSCCCO
Mol. weight [g/mol]:	106.19
CAS:	505-10-2

Physical Properties

Property code	Value	Unit	Source
gf	-120.90	kJ/mol	Joback Method
hf	-236.25	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	47.99	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.732		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
rinpol	950.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	982.00		NIST Webbook

rinpol	950.00	NIST Webbook
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ripol	1746.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1719.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1708.00		NIST Webbook
tb	451.88	K	Joback Method
tc	635.80	K	Joback Method
tf	230.06	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.56	J/mol×K	451.88	Joback Method
cpg	182.30	J/mol×K	482.53	Joback Method
cpg	189.74	J/mol×K	513.19	Joback Method
cpg	196.89	J/mol×K	543.84	Joback Method
cpg	203.75	J/mol×K	574.49	Joback Method
cpg	210.33	J/mol×K	605.15	Joback Method
cpg	216.63	J/mol×K	635.80	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.70	K	1.70	NIST Webbook

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=C505102&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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