

4-Penten-2-ol, 5-(methylthio)-, (Z)-

Other names:	5-(Methylthio)-4-penten-2-ol
Inchi:	InChI=1S/C6H12OS/c1-6(7)4-3-5-8-2/h3,5-7H,4H2,1-2H3/b5-3+
InchiKey:	IIITWVBSNBEZHT-HWKANZROSA-N
Formula:	C6H12OS
SMILES:	CSC=CCC(C)O
Mol. weight [g/mol]:	132.22
CAS:	97369-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-26.28	kJ/mol	Joback Method
hf	-165.59	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	52.02	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.634		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
ripol	1659.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	501.36	K	Joback Method
tc	693.99	K	Joback Method
tf	232.52	K	Joback Method
vc	0.418	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.17	J/molxK	501.36	Joback Method
cpg	247.02	J/molxK	533.46	Joback Method
cpg	256.38	J/molxK	565.57	Joback Method
cpg	265.27	J/molxK	597.67	Joback Method
cpg	273.71	J/molxK	629.78	Joback Method
cpg	281.72	J/molxK	661.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97369794&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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