

2-Methyl-3-(methylthio)-1-propene

Inchi:	InChI=1S/C5H10S/c1-5(2)4-6-3/h1,4H2,2-3H3
InchiKey:	OFSJHBMVJFGCIG-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	C=C(C)CSC
Mol. weight [g/mol]:	102.20
CAS:	52326-10-0

Physical Properties

Property code	Value	Unit	Source
gf	103.63	kJ/mol	Joback Method
hf	10.98	kJ/mol	Joback Method
hfus	10.25	kJ/mol	Joback Method
hvap	32.95	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.925		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	379.14	K	Joback Method
tc	577.60	K	Joback Method
tf	164.79	K	Joback Method
vc	0.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.71	J/mol×K	379.14	Joback Method
cpg	165.22	J/mol×K	412.22	Joback Method
cpg	174.32	J/mol×K	445.29	Joback Method
cpg	183.03	J/mol×K	478.37	Joback Method
cpg	191.35	J/mol×K	511.45	Joback Method
cpg	199.30	J/mol×K	544.52	Joback Method
cpg	206.88	J/mol×K	577.60	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=C52326100&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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