2-Methyl-3-butene-2-thiol

Other names: 2-Methyl-2-buten-1-thiol
Inchi: InChI=1S/C5H10S/c1-3-5(2)4-6/h3,6H,4H2,1-2H3/b5-3+
InchiKey: ZKDRFRZNMQYWPD-HWKANZROSA-N
Formula: C5H10S
SMILES: CC=C(C)CS
Mol. weight [g/mol]: 102.20

Physical Properties

Property code	Value	Unit	Source
gf	92.28	kJ/mol	Joback Method
hf	-0.62	kJ/mol	Joback Method
hfus	11.64	kJ/mol	Joback Method
hvap	33.50	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.882		Crippen Method
mcvol	93.360	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
tb	380.70	K	Joback Method
tc	585.16	K	Joback Method
tf	163.53	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.62	J/mol×K	380.70	Joback Method
cpg	163.54	J/mol×K	414.78	Joback Method
cpg	172.94	J/mol×K	448.85	Joback Method
cpg	181.82	J/mol×K	482.93	Joback Method
cpg	190.23	J/mol×K	517.01	Joback Method
cpg	198.18	J/mol×K	551.09	Joback Method
cpg	205.70	J/mol×K	585.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U99454&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume