3-Methyl-2-butene-1-thiol

Other names:	3-Methyl-2-buten-1-thiol
	3-Methyl-2-butenethiol
	3-Methyl-but-2-ene-1-thiol
	Prenyl mercaptan
	Prenylthiol
	3-methyl-2-butene-1-thiol (isopentenylmercaptan)
	2-Butene-1-thiol, 3-methyl-
	3-methylsulfanylhexyl acetate
Inchi:	InChI=1S/C5H10S/c1-5(2)3-4-6/h3,6H,4H2,1-2H3
InchiKey:	GYDPOKGOQFTYGW-UHFFFAOYSA-N
Formula:	C5H10S
SMILES:	CC(C)=CCS
Mol. weight [g/mol]:	102.20
CAS:	5287-45-6

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	804.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	808.00		NIST Webbook

rinpol	833.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	818.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1111.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1098.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1122.00		NIST Webbook
ripol	1111.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1098.00		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=C5287456&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume