

3-Mercapto-3-methyl-1-butanol

Inchi:	InChI=1S/C5H12OS/c1-5(2,7)3-4-6/h6-7H,3-4H2,1-2H3
InchiKey:	GBCGIJAYTBMFHI-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CC(C)(S)CCO
Mol. weight [g/mol]:	120.21

Physical Properties

Property code	Value	Unit	Source
gf	-113.37	kJ/mol	Joback Method
hf	-269.03	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	48.84	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.077		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	972.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	465.61	K	Joback Method
tc	659.33	K	Joback Method
tf	245.81	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.31	J/mol×K	465.61	Joback Method
cpg	225.15	J/mol×K	497.90	Joback Method
cpg	234.43	J/mol×K	530.18	Joback Method
cpg	243.17	J/mol×K	562.47	Joback Method
cpg	251.41	J/mol×K	594.76	Joback Method

cpg	259.16	J/mol×K	627.05	Joback Method
cpg	266.46	J/mol×K	659.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R598880&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

Latest version available from:

<https://www.chemeo.com/cid/71-933-7/3-Mercapto-3-methyl-1-butanol.pdf>

Generated by Cheméo on 2025-12-05 15:01:28.895260101 +0000 UTC m=+4695086.425300765.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.