

Acetic acid, 3-mercapto-3-methylbutyl ester

Other names:	3-Methyl-3-sulfanylbutyl Acetate 3-mercapto-3-methylbutyl- acetate
Inchi:	InChI=1S/C7H14O2S/c1-6(8)9-5-4-7(2,3)10/h10H,4-5H2,1-3H3
InchiKey:	HEZWKNVLHZGPOE-UHFFFAOYSA-N
Formula:	C7H14O2S
SMILES:	CC(=O)OCCC(C)(C)S
Mol. weight [g/mol]:	162.25

Physical Properties

Property code	Value	Unit	Source
gf	-193.63	kJ/mol	Joback Method
hf	-402.88	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.648		Crippen Method
mcvol	133.280	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	495.48	K	Joback Method
tc	705.11	K	Joback Method
tf	279.69	K	Joback Method
vc	0.494	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.83	J/mol×K	495.48	Joback Method
cpg	301.62	J/mol×K	530.42	Joback Method

cpg	313.72	J/mol×K	565.36	Joback Method
cpg	325.14	J/mol×K	600.30	Joback Method
cpg	335.90	J/mol×K	635.23	Joback Method
cpg	346.04	J/mol×K	670.17	Joback Method
cpg	355.57	J/mol×K	705.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U314314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvac:	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:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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