

3-Mercapto-3-methylbutyl formate (ester)

Other names:	3-Mercapto-3-methylbutyl formate Formic acid 3-mercapto-3-methyl-butyl ester
Inchi:	InChI=1S/C6H12O2S/c1-6(2,9)3-4-8-5-7/h5,9H,3-4H2,1-2H3
InchiKey:	VTAPYUYITKYXJB-UHFFFAOYSA-N
Formula:	C6H12O2S
SMILES:	CC(C)(S)CCOC=O
Mol. weight [g/mol]:	148.22
CAS:	50746-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-172.65	kJ/mol	Joback Method
hf	-355.24	kJ/mol	Joback Method
hfus	11.40	kJ/mol	Joback Method
hvap	43.52	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.258		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1027.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1507.00		NIST Webbook
tb	467.39	K	Joback Method
tc	674.54	K	Joback Method
tf	260.49	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.56	J/mol×K	467.39	Joback Method
cpg	259.88	J/mol×K	501.91	Joback Method
cpg	270.60	J/mol×K	536.44	Joback Method
cpg	280.72	J/mol×K	570.96	Joback Method
cpg	290.26	J/mol×K	605.49	Joback Method
cpg	299.25	J/mol×K	640.01	Joback Method
cpg	307.71	J/mol×K	674.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50746106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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

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