

3-Mercaptobutanal

Inchi:	InChI=1S/C4H8OS/c1-4(6)2-3-5/h3-4,6H,2H2,1H3
InchiKey:	USJRMLZTONLKON-UHFFFAOYSA-N
Formula:	C4H8OS
SMILES:	CC(S)CC=O
Mol. weight [g/mol]:	104.17

Physical Properties

Property code	Value	Unit	Source
gf	-89.77	kJ/mol	Joback Method
hf	-178.27	kJ/mol	Joback Method
hfus	8.92	kJ/mol	Joback Method
hvap	37.57	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.894		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpola	803.00		NIST Webbook
rinpola	803.00		NIST Webbook
rinpola	803.00		NIST Webbook
tb	402.00	K	Joback Method
tc	606.28	K	Joback Method
tf	198.30	K	Joback Method
vc	0.325	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.49	J/molxK	402.00	Joback Method
cpg	157.46	J/molxK	436.05	Joback Method
cpg	165.07	J/molxK	470.09	Joback Method
cpg	172.31	J/molxK	504.14	Joback Method
cpg	179.19	J/molxK	538.18	Joback Method
cpg	185.73	J/molxK	572.23	Joback Method
cpg	191.94	J/molxK	606.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R602692&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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