

Diacetyl sulphide

Other names:	1,1'-Thiobis-(ethane-1-one) (CH3CO)2S Acetyl sulfide Ethanethioic acid, anhydrosulfide acetic thioanhydride
Inchi:	InChI=1S/C4H6O2S/c1-3(5)7-4(2)6/h1-2H3
InchiKey:	DPCQJLQPDJPRCM-UHFFFAOYSA-N
Formula:	C4H6O2S
SMILES:	CC(=O)SC(C)=O
Mol. weight [g/mol]:	118.15
CAS:	3232-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-241.92	kJ/mol	Joback Method
hf	-317.00 ± 10.00	kJ/mol	NIST Webbook
hfus	13.44	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	0.813		Crippen Method
mcvol	86.710	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	392.70	K	NIST Webbook
tc	684.84	K	Joback Method
tf	269.10	K	Joback Method
vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.19	J/mol×K	612.37	Joback Method
cpg	191.15	J/mol×K	648.60	Joback Method
cpg	157.86	J/mol×K	467.44	Joback Method
cpg	165.20	J/mol×K	503.67	Joback Method

cpg	172.21	J/mol×K	539.91	Joback Method
cpg	178.87	J/mol×K	576.14	Joback Method
cpg	196.77	J/mol×K	684.84	Joback Method
hvapt	54.20	kJ/mol	340.00	NIST Webbook
hvapt	50.90	kJ/mol	340.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C3232391&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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