

Benzaldehyde, 4-(methylthio)-

Other names:	p-(Methylthio)benzaldehyde p-Methylmercaptobenzaldehyde 4-(methylthio)benzaldehyde
Inchi:	InChI=1S/C8H8OS/c1-10-8-4-2-7(6-9)3-5-8/h2-6H,1H3
InchiKey:	QRVYABWJVXXOTN-UHFFFAOYSA-N
Formula:	C8H8OS
SMILES:	CSc1ccc(C=O)cc1
Mol. weight [g/mol]:	152.21
CAS:	3446-89-7

Physical Properties

Property code	Value	Unit	Source
gf	52.86	kJ/mol	Joback Method
hf	-27.10	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.221		Crippen Method
mcvol	117.740	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	531.54	K	Joback Method
tc	771.23	K	Joback Method
tf	295.26	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.38	J/mol×K	531.54	Joback Method
cpg	249.66	J/mol×K	571.49	Joback Method
cpg	260.18	J/mol×K	611.44	Joback Method
cpg	269.98	J/mol×K	651.38	Joback Method
cpg	279.08	J/mol×K	691.33	Joback Method
cpg	287.49	J/mol×K	731.28	Joback Method

cpg

295.24

J/mol×K

771.23

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	0.10	NIST Webbook

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=C3446897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/39-783-0/Benzaldehyde-4-methylthio.pdf>

Generated by Cheméo on 2025-12-18 17:24:37.750252819 +0000 UTC m=+5826875.280293474.

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