Benzaldehyde, p-methoxythio-

Inchi: InChI=1S/C8H8OS/c1-9-8-4-2-7(6-10)3-5-8/h2-6H,1H3
InchiKey: PSCGHQRKTJYCJO-UHFFFAOYSA-N
Formula: C8H8OS
SMILES: COc1ccc(C=S)cc1
Mol. weight [g/mol]: 152.21
CAS: 25332-53-0

Physical Properties

Property code	Value	Unit	Source
gf	139.87	kJ/mol	Joback Method
hf	40.68	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	45.40	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.043		Crippen Method
mcvol	117.740	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	506.68	K	Joback Method
tc	741.53	K	Joback Method
tf	289.32	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.83	J/mol×K	506.68	Joback Method
cpg	239.91	J/mol×K	545.82	Joback Method
cpg	250.21	J/mol×K	584.96	Joback Method
cpg	259.78	J/mol×K	624.11	Joback Method
cpg	268.67	J/mol×K	663.25	Joback Method
cpg	276.93	J/mol×K	702.39	Joback Method
cpg	284.61	J/mol×K	741.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C25332530&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
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