Benzenecarbothioic acid, S-methyl ester

Other names:	Benzoic acid, thio-, S-methyl ester
	S-Methyl thiobenzoate
	Thiobenzoic acid S-methyl ester
	Methyl thiobenzoate
Inchi:	InChI=1S/C8H8OS/c1-10-8(9)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	RQVWTMCUTHKGCM-UHFFFAOYSA-N
Formula:	C8H8OS
SMILES:	CSC(=O)c1ccccc1
Mol. weight [g/mol]:	152.21
CAS:	5925-68-8

Physical Properties

Property code	Value	Unit	Source
gf	33.09	kJ/mol	Joback Method
hf	-42.63	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.190		Crippen Method
mcvol	117.740	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	1298.60		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1295.00		NIST Webbook
tb	531.77	K	Joback Method
tc	776.43	K	Joback Method
tf	290.67	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.47	J/mol×K	531.77	Joback Method
cpg	249.47	J/mol×K	572.55	Joback Method

cpg	260.61	J/mol×K	613.32	Joback Method
cpg	270.92	J/mol×K	654.10	Joback Method
cpg	280.43	J/mol×K	694.88	Joback Method
cpg	289.16	J/mol×K	735.65	Joback Method
cpg	297.16	J/mol×K	776.43	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=C5925688&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume