Benzoic acid, o-mercapto-, methyl ester

Inchi: InChI=1S/C8H8O2S/c1-10-8(9)6-4-2-3-5-7(6)11/h2-5,11H,1H3
InchiKey: BAQGCWNPCFABAY-UHFFFAOYSA-N
Formula: C8H8O2S
SMILES: COC(=O)c1ccccc1S
Mol. weight [g/mol]: 168.21
CAS: 4892-02-8

Physical Properties

Property code	Value	Unit	Source
gf	-85.27	kJ/mol	Joback Method
hf	-189.71	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.762		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	553.25	K	Joback Method
tc	796.12	K	Joback Method
tf	327.48	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.77	J/mol×K	553.25	Joback Method
cpg	268.10	J/mol×K	593.73	Joback Method
cpg	278.70	J/mol×K	634.21	Joback Method
cpg	288.59	J/mol×K	674.68	Joback Method
cpg	297.78	J/mol×K	715.16	Joback Method
cpg	306.27	J/mol×K	755.64	Joback Method
cpg	314.07	J/mol×K	796.12	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=C4892028&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