Benzoic acid, 3-mercapto-

Other names: 3-Mercaptobenzoic acid
Inchi: InChI=1S/C7H6O2S/c8-7(9)5-2-1-3-6(10)4-5/h1-4,10H,(H,8,9)
InchiKey: RSFDFESMVAIVKO-UHFFFAOYSA-N
Formula: C7H6O2S
SMILES: O=C(O)c1cccc(S)c1
Mol. weight [g/mol]: 154.19
CAS: 4869-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-125.51	kJ/mol	Joback Method
hf	-189.08	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	64.28	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.673		Crippen Method
mcvol	109.520	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	600.13	K	Joback Method
tc	829.79	K	Joback Method
tf	354.80	K	Joback Method
vc	0.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.89	J/mol×K	600.13	Joback Method
cpg	240.11	J/mol×K	638.41	Joback Method
cpg	247.73	J/mol×K	676.68	Joback Method
cpg	254.78	J/mol×K	714.96	Joback Method
cpg	261.28	J/mol×K	753.24	Joback Method
cpg	267.27	J/mol×K	791.51	Joback Method

cpg	272.77	J/mol×K	829.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4869594&Units=SI
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

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