Benzoic acid, 2-mercapto-

Other names:	Benzoic acid, o-mercapto-
	o-Benzoic acid thiol
	o-Mercaptobenzoic acid
	o-Sulfhydrylbenzoic acid
	o-Thiosalicylic acid
	Salicylic acid, 2-thio-
	2-Carboxythiophenol
	2-Mercaptobenzoic acid
	Thiosalicylic acid
	o-Mercaptobenzoesaeure
	USAF EK-T-2805
	USAF KF-2
	USAF XR-35
	o-Carboxythiophenol
	Thiophenol-2-carboxylic acid
	2-Thiosalicylic acid
	NSC 2184
	NSC 660640
	2-Sulfanylbenzoic acid
	860499-02-1
Inchi:	InChI=1S/C7H6O2S/c8-7(9)5-3-1-2-4-6(5)10/h1-4,10H,(H,8,9)
InchiKey:	NBOMNTLFRHMDEZ-UHFFFAOYSA-N
Formula:	C7H6O2S
SMILES:	O=C(O)c1ccccc1S
Mol. weight [g/mol]:	154.19
CAS:	147-93-3

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	1494.00		NIST Webbook
rinpol	1497.00		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

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=C147933&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume