4-MERCAPTOBENZOIC ACID

Other names: Benzoic acid, p-mercapto-
4-Carboxybenzenethiol
4-Mercaptobenzoic acid
p-Mercaptobenzoic acid
4-Sulfanylbenzoic acid
Inchi: InChI=1S/C7H6O2S/c8-7(9)5-1-3-6(10)4-2-5/h1-4,10H,(H,8,9)
InchiKey: LMJXSOYPAOSIPZ-UHFFFAOYSA-N
Formula: C7H6O2S
SMILES: O=C(O)c1ccc(S)cc1
Mol. weight [g/mol]: 154.19

Physical Properties

Property code	Value	Unit	Source
af	0.6552		Cheméo Relay (1.0)
gf	-125.51	kJ/mol	Joback Method
hf	-282.78	kJ/mol	Cheméo Relay (1.0)
hfus	17.27	kJ/mol	Joback Method
hvap	101.55	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	1.673		Crippen Method
mcvol	109.520	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
rinpol	1503.00		NIST Webbook
tb	576.97	K	Cheméo Relay (1.0)
tc	826.96	K	Cheméo Relay (1.0)
tf	485.58	K	Cheméo Relay (1.0)
vc	0.357	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074368&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
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
ie: Ionization energy
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.