2-Sulfobenzoic acid cyclic anhydride

Other names:	2-Sulfobenzoic anhydride
	o-Sulfobenzoic anhydride
	o-Sulfobenzoic acid cyclic anhydride
	3H-2,1-Benzoxathiol-3-one, 1,1-dioxide
	o-Sulfobenzoic acid anhydride
	Benzoic acid, o-sulfo-, cyclic anhydride
	Benzoic acid, 2-sulfo-, cyclic anhydride
	Sulfobenzoic anhydride
	NSC 11208
	2-sulphobenzoic anhydride
Inchi:	InChI=1S/C7H4O4S/c8-7-5-3-1-2-4-6(5)12(9,10)11-7/h1-4H
InchiKey:	NCYNKWQXFADUOZ-UHFFFAOYSA-N
Formula:	C7H4O4S
SMILES:	O=C1OS(=O)(=O)c2ccccc21
Mol. weight [g/mol]:	184.17
CAS:	81-08-3

Physical Properties

Property code	Value	Unit	Source
gf	-491.21	kJ/mol	Joback Method
hf	-589.27	kJ/mol	Joback Method
hfus	23.00	kJ/mol	Joback Method
hvap	60.72	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	0.546		Crippen Method
mcvol	110.400	ml/mol	McGowan Method
pc	6369.39	kPa	Joback Method
tb	524.23	K	Joback Method
tc	756.88	K	Joback Method
tf	412.17	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.47	J/mol×K	524.23	Joback Method
cpg	246.12	J/mol×K	563.00	Joback Method
cpg	256.05	J/mol×K	601.78	Joback Method
cpg	265.25	J/mol×K	640.55	Joback Method
cpg	273.75	J/mol×K	679.33	Joback Method
cpg	281.57	J/mol×K	718.10	Joback Method
cpg	288.73	J/mol×K	756.88	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81083&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

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