

C7H8O3S

Inchi:	InChI=1S/C7H8O3S/c1-11(9,10)7-4-2-6(8)3-5-7/h2-5,8H,1H3
InchiKey:	KECCFSZFXLAGJS-UHFFFAOYSA-N
Formula:	C7H8O3S
SMILES:	CS(=O)(=O)c1ccc(O)cc1
Mol. weight [g/mol]:	172.20
CAS:	14763-60-1

Physical Properties

Property code	Value	Unit	Source
gf	-502.69	kJ/mol	Joback Method
hf	-581.94	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	65.10	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.796		Crippen Method
mcvol	119.690	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
tb	514.64	K	Joback Method
tc	735.73	K	Joback Method
tf	345.35	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.88	J/mol×K	514.64	Joback Method
cpg	268.07	J/mol×K	551.49	Joback Method
cpg	278.44	J/mol×K	588.34	Joback Method
cpg	288.04	J/mol×K	625.18	Joback Method
cpg	296.92	J/mol×K	662.03	Joback Method
cpg	305.14	J/mol×K	698.88	Joback Method
cpg	312.73	J/mol×K	735.73	Joback Method

Sources

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=C14763601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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

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