

2,5-Thiophenedicarboxylic acid

Other names:	2,5-Dicarboxythiophene thiophene-2,5-dicarboxylic acid
Inchi:	InChI=1S/C6H4O4S/c7-5(8)3-1-2-4(11-3)6(9)10/h1-2H,(H,7,8)(H,9,10)
InchiKey:	YCGAZNXXGKTASZ-UHFFFAOYSA-N
Formula:	C6H4O4S
SMILES:	O=C(O)c1ccc(C(=O)O)s1
Mol. weight [g/mol]:	172.16
CAS:	4282-31-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	1.145		Crippen Method
mvol	107.170	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	161.40	J/molxK	277.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	162.70	J/molxK	280.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	163.70	J/molxK	285.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives

cps	164.70	J/mol×K	290.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	166.40	J/mol×K	295.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	167.10	J/mol×K	298.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	167.70	J/mol×K	300.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	169.50	J/mol×K	305.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	171.00	J/mol×K	310.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	173.10	J/mol×K	315.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	175.10	J/mol×K	320.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	177.00	J/mol×K	325.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives

cps	178.10	J/mol×K	330.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	179.70	J/mol×K	335.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	180.80	J/mol×K	340.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	182.30	J/mol×K	345.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	184.00	J/mol×K	350.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	186.10	J/mol×K	355.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	186.40	J/mol×K	360.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	190.10	J/mol×K	365.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives

cps	192.40	J/mol×K	370.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	194.20	J/mol×K	375.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	196.70	J/mol×K	380.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	198.70	J/mol×K	385.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	200.90	J/mol×K	390.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	203.30	J/mol×K	395.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	206.10	J/mol×K	400.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	209.60	J/mol×K	405.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	210.90	J/mol×K	410.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives

cps	213.70	J/molxK	415.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	216.30	J/molxK	420.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	219.40	J/molxK	425.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	223.10	J/molxK	430.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	225.50	J/molxK	435.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	228.10	J/molxK	440.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives
cps	229.80	J/molxK	445.15	Thermophysical properties of sulfur heterocycles: Thiane and thiophene derivatives

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4282319&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Solid-liquid equilibrium and thermodynamic of 2-thiophenedicarboxylic acid in determination of the solid-liquid equilibrium physical properties of sulfur heterocycles: Thiophene and thiothene Solubility and solution thermodynamics of 2-thiophenedicarboxylic acid in (water + ethanol) binary solvent mixtures:

<https://www.doi.org/10.1016/j.fluid.2014.05.003>

<https://www.doi.org/10.1016/j.fluid.2015.06.007>

<https://www.doi.org/10.1016/j.tca.2005.11.024>

<https://www.doi.org/10.1016/j.tca.2014.08.002>

<http://link.springer.com/article/10.1007/BF02311772>

Legend

cps: Solid phase heat capacity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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