

# Asparagusic acid

<b>Inchi:</b>	InChI=1S/C4H6O2S2/c5-4(6)3-1-7-8-2-3/h3H,1-2H2,(H,5,6)
<b>InchiKey:</b>	AYGMEFRECNRJJC-UHFFFAOYSA-N
<b>Formula:</b>	C4H6O2S2
<b>SMILES:</b>	O=C(O)C1CSSC1
<b>Mol. weight [g/mol]:</b>	150.22
<b>CAS:</b>	2224-02-4

## Physical Properties

Property code	Value	Unit	Source
gf	-166.67	kJ/mol	Joback Method
hf	-239.70	kJ/mol	Joback Method
hfus	13.05	kJ/mol	Joback Method
hvap	59.80	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.082		Crippen Method
mvol	96.500	ml/mol	McGowan Method
pc	6113.06	kPa	Joback Method
rinpol	1444.20		NIST Webbook
rinpol	1444.20		NIST Webbook
tb	547.91	K	Joback Method
tc	777.20	K	Joback Method
tf	423.39	K	Joback Method
vc	0.318	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.92	J/mol×K	547.91	Joback Method
cpg	209.38	J/mol×K	586.12	Joback Method
cpg	217.24	J/mol×K	624.34	Joback Method
cpg	224.54	J/mol×K	662.55	Joback Method
cpg	231.30	J/mol×K	700.77	Joback Method
cpg	237.56	J/mol×K	738.98	Joback Method
cpg	243.34	J/mol×K	777.20	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2224024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2224024&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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