

# Anthralic acid, 6-fluoro-

<b>Other names:</b>	2-Amino-6-fluorobenzoic acid
<b>Inchi:</b>	InChI=1S/C7H6FNO2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,9H2,(H,10,11)
<b>InchiKey:</b>	RWSFZKWMVWPDGZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H6FNO2
<b>SMILES:</b>	<chem>Nc1cccc(F)c1C(=O)O</chem>
<b>Mol. weight [g/mol]:</b>	155.13
<b>CAS:</b>	434-76-4

## Physical Properties

Property code	Value	Unit	Source
gf	-292.89	kJ/mol	Joback Method
hf	-401.35	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.106		Crippen Method
mcvol	104.920	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
tb	614.05	K	Joback Method
tc	823.95	K	Joback Method
tf	414.71	K	Joback Method
vc	0.392	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.86	J/molxK	614.05	Joback Method
cpg	254.46	J/molxK	649.03	Joback Method
cpg	261.57	J/molxK	684.02	Joback Method
cpg	268.22	J/molxK	719.00	Joback Method
cpg	274.41	J/molxK	753.98	Joback Method
cpg	280.17	J/molxK	788.97	Joback Method
cpg	285.50	J/molxK	823.95	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C434764&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C434764&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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