

# 2,6-Difluorobenzoic acid

<b>Other names:</b>	Benzoic acid, 2,6-difluoro-
<b>Inchi:</b>	InChI=1S/C7H4F2O2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H,10,11)
<b>InchiKey:</b>	ONOTYLMNTZNAQZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H4F2O2
<b>SMILES:</b>	O=C(O)c1c(F)cccc1F
<b>Mol. weight [g/mol]:</b>	158.10
<b>CAS:</b>	385-00-2

## Physical Properties

Property code	Value	Unit	Source
gf	-554.15	kJ/mol	Joback Method
hf	-631.25	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.663		Crippen Method
mcvol	96.710	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	540.79	K	Joback Method
tc	732.76	K	Joback Method
tf	332.04	K	Joback Method
vc	0.381	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.83	J/mol×K	540.79	Joback Method
cpg	215.99	J/mol×K	572.79	Joback Method
cpg	222.74	J/mol×K	604.78	Joback Method
cpg	229.10	J/mol×K	636.78	Joback Method
cpg	235.09	J/mol×K	668.77	Joback Method
cpg	240.70	J/mol×K	700.77	Joback Method
cpg	245.97	J/mol×K	732.76	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C385002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C385002&amp;Units=SI</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>hvap:</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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