

# 1-Propanone, 1-(2,4-difluorophenyl)-

<b>Other names:</b>	2,5-Difluoropropiophenone 2,4-Difluoropropiophenone 2',4'-difluoropropiophenone
<b>Inchi:</b>	InChI=1S/C9H8F2O/c1-2-9(12)7-4-3-6(10)5-8(7)11/h3-5H,2H2,1H3
<b>InchiKey:</b>	UZWOADNMVRRYDE-UHFFFAOYSA-N
<b>Formula:</b>	C9H8F2O
<b>SMILES:</b>	CCC(=O)c1ccc(F)cc1F
<b>Mol. weight [g/mol]:</b>	170.16
<b>CAS:</b>	85068-30-0

## Physical Properties

Property code	Value	Unit	Source
gf	-400.49	kJ/mol	Joback Method
hf	-520.30	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.558		Crippen Method
mcvol	119.020	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	494.37	K	Joback Method
tc	693.12	K	Joback Method
tf	293.76	K	Joback Method
vc	0.473	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.27	J/molxK	494.37	Joback Method
cpg	261.17	J/molxK	527.50	Joback Method
cpg	271.50	J/molxK	560.62	Joback Method
cpg	281.27	J/molxK	593.75	Joback Method
cpg	290.51	J/molxK	626.87	Joback Method
cpg	299.22	J/molxK	660.00	Joback Method

## Sources

<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=C85068300&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85068300&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>

## 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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