

# 2,6-Difluorobenzoic acid, 3,5-difluorophenyl ester

<b>Inchi:</b>	InChI=1S/C13H6F4O2/c14-7-4-8(15)6-9(5-7)19-13(18)12-10(16)2-1-3-11(12)17/h1-6H
<b>InchiKey:</b>	AOODVHZSRUNYDJ-UHFFFAOYSA-N
<b>Formula:</b>	C13H6F4O2
<b>SMILES:</b>	O=C(Oc1cc(F)cc(F)c1)c1c(F)cccc1F
<b>Mol. weight [g/mol]:</b>	270.18

## Physical Properties

Property code	Value	Unit	Source
gf	-768.28	kJ/mol	Joback Method
hf	-913.71	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	57.62	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.462		Crippen Method
mvol	161.030	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1547.30		NIST Webbook
rinpol	1547.30		NIST Webbook
tb	643.49	K	Joback Method
tc	852.13	K	Joback Method
tf	413.71	K	Joback Method
vc	0.643	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.83	J/mol×K	643.49	Joback Method
cpg	406.05	J/mol×K	678.26	Joback Method
cpg	416.52	J/mol×K	713.04	Joback Method
cpg	426.28	J/mol×K	747.81	Joback Method
cpg	435.32	J/mol×K	782.58	Joback Method
cpg	443.67	J/mol×K	817.36	Joback Method
cpg	451.33	J/mol×K	852.13	Joback Method

# Sources

<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=U292621&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292621&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpola:</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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