

# 2,5-Difluorobenzoic acid, 4-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C13H7ClF2O2/c14-8-1-4-10(5-2-8)18-13(17)11-7-9(15)3-6-12(11)16/h1-7H
<b>InchiKey:</b>	ZZSJFXRNCMVQCY-UHFFFAOYSA-N
<b>Formula:</b>	C13H7ClF2O2
<b>SMILES:</b>	O=C(Oc1ccc(Cl)cc1)c1cc(F)ccc1F
<b>Mol. weight [g/mol]:</b>	268.64

## Physical Properties

Property code	Value	Unit	Source
gf	-380.96	kJ/mol	Joback Method
hf	-525.76	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.837		Crippen Method
mcvol	169.730	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinsol	1851.00		NIST Webbook
tb	677.40	K	Joback Method
tc	908.05	K	Joback Method
tf	429.93	K	Joback Method
vc	0.656	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.10	J/mol×K	677.40	Joback Method
cpg	414.64	J/mol×K	715.84	Joback Method
cpg	425.29	J/mol×K	754.28	Joback Method
cpg	435.06	J/mol×K	792.72	Joback Method
cpg	443.98	J/mol×K	831.16	Joback Method
cpg	452.08	J/mol×K	869.61	Joback Method
cpg	459.38	J/mol×K	908.05	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=U357580&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357580&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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