

# 2-butenyl pentafluorobenzoate

<b>Inchi:</b>	InChI=1S/C11H7F5O2/c1-2-3-4-18-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h2-3H,4H2,1H3
<b>InchiKey:</b>	RJSCWKIHRDEMFX-NSCUHMNNSA-N
<b>Formula:</b>	C11H7F5O2
<b>SMILES:</b>	CC=CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	266.16

## Physical Properties

Property code	Value	Unit	Source
gf	-1021.75	kJ/mol	Joback Method
hf	-1199.32	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.115		Crippen Method
mcvol	154.080	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
ripol	1207.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1205.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1198.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1548.00		NIST Webbook
ripol	1583.00		NIST Webbook
tb	579.46	K	Joback Method
tc	757.46	K	Joback Method
tf	372.78	K	Joback Method
vc	0.637	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.48	J/mol×K	579.46	Joback Method
cpg	375.26	J/mol×K	609.13	Joback Method
cpg	384.61	J/mol×K	638.79	Joback Method
cpg	393.53	J/mol×K	668.46	Joback Method
cpg	402.02	J/mol×K	698.13	Joback Method
cpg	410.10	J/mol×K	727.79	Joback Method
cpg	417.75	J/mol×K	757.46	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R311856&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R311856&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.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>

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	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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