

# C7H6F6O2

<b>Inchi:</b>	InChI=1S/C7H6F6O2/c1-2-15-5(14)3-4(6(8,9)10)7(11,12)13/h3H,2H2,1H3
<b>InchiKey:</b>	CULZFNOUNPBWSIZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H6F6O2
<b>SMILES:</b>	CCOC(=O)C=C(C(F)(F)F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	236.11
<b>CAS:</b>	1513-60-6

## Physical Properties

Property code	Value	Unit	Source
gf	-1317.37	kJ/mol	Joback Method
hf	-1519.34	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	32.88	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.601		Crippen Method
mcvol	123.250	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
tb	429.05	K	Joback Method
tc	585.62	K	Joback Method
tf	230.15	K	Joback Method
vc	0.518	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.30	J/molxK	429.05	Joback Method
cpg	287.47	J/molxK	455.14	Joback Method
cpg	297.04	J/molxK	481.24	Joback Method
cpg	306.05	J/molxK	507.33	Joback Method
cpg	314.52	J/molxK	533.43	Joback Method
cpg	322.48	J/molxK	559.52	Joback Method
cpg	329.94	J/molxK	585.62	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=C1513606&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1513606&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>
<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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