

# «alpha», «alpha», «alpha», 2,3,5,6-Heptafluoro-p-xy

<b>Inchi:</b>	InChI=1S/C8H3F7/c1-2-4(9)6(11)3(8(13,14)15)7(12)5(2)10/h1H3
<b>InchiKey:</b>	JBZHWNXMZYBXDQ-UHFFFAOYSA-N
<b>Formula:</b>	C8H3F7
<b>SMILES:</b>	Cc1c(F)c(F)c(C(F)(F)F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	232.10
<b>CAS:</b>	778-35-8

## Physical Properties

Property code	Value	Unit	Source
gf	-1280.09	kJ/mol	Joback Method
hf	-1410.79	kJ/mol	Joback Method
hfus	22.72	kJ/mol	Joback Method
hvap	31.97	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.570		Crippen Method
mcvol	112.210	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	417.20	K	NIST Webbook
tc	584.82	K	Joback Method
tf	275.49	K	Joback Method
vc	0.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.02	J/mol×K	425.68	Joback Method
cpg	249.12	J/mol×K	452.20	Joback Method
cpg	256.85	J/mol×K	478.73	Joback Method
cpg	264.22	J/mol×K	505.25	Joback Method
cpg	271.25	J/mol×K	531.77	Joback Method
cpg	277.93	J/mol×K	558.30	Joback Method
cpg	284.29	J/mol×K	584.82	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C778358&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C778358&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>
<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>mccvol:</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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