

# p-Fluoro-«alpha»,«alpha»,«alpha»-trichlorotoluene

Inchi:	InChI=1S/C7H4Cl3F/c8-7(9,10)5-1-3-6(11)4-2-5/h1-4H
InchiKey:	XOJYLEJZALFLLW-UHFFFAOYSA-N
Formula:	C7H4Cl3F
SMILES:	Fc1ccc(C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]:	213.46
CAS:	402-42-6

## Physical Properties

Property code	Value	Unit	Source
gf	-116.92	kJ/mol	Joback Method
hf	-214.83	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	45.16	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.652		Crippen Method
mcvol	124.220	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	1181.10		NIST Webbook
rinpol	1181.10		NIST Webbook
tb	499.55	K	Joback Method
tc	736.18	K	Joback Method
tf	300.36	K	Joback Method
vc	0.473	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.81	J/mol×K	499.55	Joback Method
cpg	230.24	J/mol×K	538.99	Joback Method
cpg	238.80	J/mol×K	578.43	Joback Method
cpg	246.53	J/mol×K	617.86	Joback Method
cpg	253.51	J/mol×K	657.30	Joback Method
cpg	259.80	J/mol×K	696.74	Joback Method
cpg	265.47	J/mol×K	736.18	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C402426&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C402426&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>hvp:</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>rinp:</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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