

# Fumaric acid, 2,5-dichlorophenyl 2,2,3,3-tetrafluoropropyl ester

**Inchi:** InChI=1S/C13H8Cl2F4O4/c14-7-1-2-8(15)9(5-7)23-11(21)4-3-10(20)22-6-13(18,19)12(16)  
**InchiKey:** HZHSICZQGXJBPQ-ONEGZZNKSA-N  
**Formula:** C13H8Cl2F4O4  
**SMILES:** O=C(C=CC(=O)Oc1cc(Cl)ccc1Cl)OCC(F)(F)C(F)F  
**Mol. weight [g/mol]:** 375.10

## Physical Properties

Property code	Value	Unit	Source
gf	-1038.59	kJ/mol	Joback Method
hf	-1300.39	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.899		Crippen Method
mcvol	212.410	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpola	1927.00		NIST Webbook
rinpola	1927.00		NIST Webbook
tb	758.49	K	Joback Method
tc	963.59	K	Joback Method
tf	476.59	K	Joback Method
vc	0.837	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.56	J/molxK	758.49	Joback Method
cpg	554.08	J/molxK	792.67	Joback Method
cpg	562.83	J/molxK	826.86	Joback Method
cpg	570.85	J/molxK	861.04	Joback Method
cpg	578.18	J/molxK	895.22	Joback Method
cpg	584.84	J/molxK	929.40	Joback Method
cpg	590.89	J/molxK	963.59	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405962&amp;Units=SI</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>rinpola:</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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