

# Succinic acid, 2-chloro-6-fluorophenyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

<b>Inchi:</b>	InChI=1S/C15H10ClF9O4/c16-7-2-1-3-8(17)11(7)29-10(27)5-4-9(26)28-6-13(20,21)15(22)
<b>InchiKey:</b>	INDNIRSZJLXTMF-UHFFFAOYSA-N
<b>Formula:</b>	C15H10ClF9O4
<b>SMILES:</b>	O=C(CCC(=O)Oc1c(F)cccc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	460.68

## Physical Properties

Property code	Value	Unit	Source
gf	-2058.41	kJ/mol	Joback Method
hf	-2441.20	kJ/mol	Joback Method
hfus	39.59	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.879		Crippen Method
mvol	241.500	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	752.55	K	Joback Method
tc	933.17	K	Joback Method
tf	482.08	K	Joback Method
vc	0.988	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.05	J/molxK	752.55	Joback Method
cpg	706.39	J/molxK	782.65	Joback Method
cpg	715.93	J/molxK	812.76	Joback Method
cpg	724.73	J/molxK	842.86	Joback Method
cpg	732.84	J/molxK	872.96	Joback Method
cpg	740.30	J/molxK	903.07	Joback Method
cpg	747.15	J/molxK	933.17	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=U390706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390706&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>

# 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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