

# Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C15H11ClF8O4/c16-8-2-1-3-9(6-8)28-11(26)5-4-10(25)27-7-13(19,20)15(23,24)
<b>InchiKey:</b>	DDNKKUKGBCGKPU-UHFFFAOYSA-N
<b>Formula:</b>	C15H11ClF8O4
<b>SMILES:</b>	O=C(CCC(=O)Oc1cccc(Cl)c1)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	442.69

## Physical Properties

Property code	Value	Unit	Source
gf	-1853.97	kJ/mol	Joback Method
hf	-2233.62	kJ/mol	Joback Method
hfus	36.90	kJ/mol	Joback Method
hvap	63.81	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.740		Crippen Method
mcvol	239.730	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	748.30	K	Joback Method
tc	932.29	K	Joback Method
tf	468.97	K	Joback Method
vc	0.970	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.56	J/mol×K	748.30	Joback Method
cpg	700.33	J/mol×K	778.97	Joback Method
cpg	710.25	J/mol×K	809.63	Joback Method
cpg	719.40	J/mol×K	840.30	Joback Method
cpg	727.81	J/mol×K	870.96	Joback Method
cpg	735.55	J/mol×K	901.63	Joback Method
cpg	742.67	J/mol×K	932.29	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U389847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U389847&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>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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