

# 3-Fluoro-4-trifluoromethylbenzoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester

<b>Inchi:</b>	InChI=1S/C12H5F11O2/c13-7-3-5(1-2-6(7)10(16,17)18)8(24)25-4-9(14,15)11(19,20)12(21,22)1
<b>InchiKey:</b>	YWRRQRYIPUQMRY-UHFFFAOYSA-N
<b>Formula:</b>	C12H5F11O2
<b>SMILES:</b>	O=C(OCC(F)(F)C(F)(F)C(F)(F)F)c1ccc(C(F)(F)F)c(F)c1
<b>Mol. weight [g/mol]:</b>	390.15

## Physical Properties

Property code	Value	Unit	Source
gf	-2222.16	kJ/mol	Joback Method
hf	-2514.43	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	40.89	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.834		Crippen Method
mcvol	183.090	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinsol	1112.00		NIST Webbook
tb	565.94	K	Joback Method
tc	725.76	K	Joback Method
tf	364.79	K	Joback Method
vc	0.777	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.91	J/molxK	565.94	Joback Method
cpg	508.07	J/molxK	592.58	Joback Method
cpg	518.41	J/molxK	619.21	Joback Method
cpg	528.00	J/molxK	645.85	Joback Method
cpg	536.88	J/molxK	672.49	Joback Method
cpg	545.08	J/molxK	699.12	Joback Method
cpg	552.67	J/molxK	725.76	Joback Method

# Sources

<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=U357348&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357348&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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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