

# 3-Fluoro-4-trifluoromethylbenzoic acid, 4-biphenyl ester

<b>Inchi:</b>	InChI=1S/C20H12F4O2/c21-18-12-15(8-11-17(18)20(22,23)24)19(25)26-16-9-6-14(7-10)
<b>InchiKey:</b>	AFZSPWLCQLHGQO-UHFFFAOYSA-N
<b>Formula:</b>	C20H12F4O2
<b>SMILES:</b>	O=C(Oc1ccc(-c2ccccc2)cc1)c1ccc(C(F)(F)F)c(F)c1
<b>Mol. weight [g/mol]:</b>	360.30

## Physical Properties

Property code	Value	Unit	Source
gf	-584.46	kJ/mol	Joback Method
hf	-818.94	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	73.52	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	5.731		Crippen Method
mcvol	235.900	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2429.00		NIST Webbook
rinpol	2429.00		NIST Webbook
tb	822.12	K	Joback Method
tc	1054.29	K	Joback Method
tf	508.92	K	Joback Method
vc	0.916	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.25	J/mol×K	822.12	Joback Method
cpg	687.00	J/mol×K	860.81	Joback Method
cpg	698.57	J/mol×K	899.51	Joback Method
cpg	709.04	J/mol×K	938.20	Joback Method
cpg	718.51	J/mol×K	976.90	Joback Method
cpg	727.06	J/mol×K	1015.59	Joback Method
cpg	734.79	J/mol×K	1054.29	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=U360602&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360602&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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