

# 4-tert-Butylcatechol, O,O'-bis(heptafluorobutyrate)

Other names:	Pyrocatechol, 4-tert.-butyl, bis-HFB
Inchi:	InChI=1S/C18H12F14O4/c1-12(2,3)7-4-5-8(35-10(33)13(19,20)15(23,24)17(27,28)29)9(
InchiKey:	BUKUNDXYDAVYCJ-UHFFFAOYSA-N
Formula:	C18H12F14O4
SMILES:	CC(C)(C)c1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]:	558.26

## Physical Properties

Property code	Value	Unit	Source
gf	-2981.47	kJ/mol	Joback Method
hf	-3497.65	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	57.06	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.461		Crippen Method
mcvol	280.380	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	1399.00		NIST Webbook
tb	767.63	K	Joback Method
tc	944.07	K	Joback Method
tf	513.60	K	Joback Method
vc	1.159	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.14	J/molxK	767.63	Joback Method
cpg	891.08	J/molxK	797.04	Joback Method
cpg	901.15	J/molxK	826.44	Joback Method
cpg	910.42	J/molxK	855.85	Joback Method
cpg	919.00	J/molxK	885.25	Joback Method
cpg	926.98	J/molxK	914.66	Joback Method
cpg	934.46	J/molxK	944.07	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=U365295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U365295&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>
<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>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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