

# Octafluoro-4,4'-biphenyldithiol

<b>Inchi:</b>	InChI=1S/C12H2F8S2/c13-3-1(4(14)8(18)11(21)7(3)17)2-5(15)9(19)12(22)10(20)6(2)16/
<b>InchiKey:</b>	BMXRSRJBWJONO-UHFFFAOYSA-N
<b>Formula:</b>	C12H2F8S2
<b>SMILES:</b>	Fc1c(F)c(-c2c(F)c(F)c(S)c(F)c2F)c(F)c(F)c1S
<b>Mol. weight [g/mol]:</b>	362.26
<b>CAS:</b>	21386-21-0

## Physical Properties

Property code	Value	Unit	Source
gf	-1321.02	kJ/mol	Joback Method
hf	-1424.57	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	5.044		Crippen Method
mcvol	179.280	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	697.00	K	Joback Method
tc	904.97	K	Joback Method
tf	480.68	K	Joback Method
vc	0.744	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.82	J/molxK	697.00	Joback Method
cpg	431.23	J/molxK	731.66	Joback Method
cpg	439.12	J/molxK	766.32	Joback Method
cpg	446.47	J/molxK	800.98	Joback Method
cpg	453.28	J/molxK	835.64	Joback Method
cpg	459.57	J/molxK	870.31	Joback Method
cpg	465.31	J/molxK	904.97	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=C21386210&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21386210&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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