

# 2,3,7,8-Tetrafluoro DBD

<b>Inchi:</b>	InChI=1S/C12H4F4O2/c13-5-1-9-10(2-6(5)14)18-12-4-8(16)7(15)3-11(12)17-9/h1-4H
<b>InchiKey:</b>	NOZDVIWMUAUYAV-UHFFFAOYSA-N
<b>Formula:</b>	C12H4F4O2
<b>SMILES:</b>	Fc1cc2c(cc1F)Oc1cc(F)c(F)cc1O2
<b>Mol. weight [g/mol]:</b>	256.15

## Physical Properties

Property code	Value	Unit	Source
gf	-653.72	kJ/mol	Joback Method
hf	-835.91	kJ/mol	Joback Method
hfus	40.03	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	4.141		Crippen Method
mcvol	140.380	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	615.32	K	Joback Method
tc	827.93	K	Joback Method
tf	434.16	K	Joback Method
vc	0.572	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.22	J/mol×K	615.32	Joback Method
cpg	354.82	J/mol×K	650.76	Joback Method
cpg	363.74	J/mol×K	686.19	Joback Method
cpg	372.05	J/mol×K	721.63	Joback Method
cpg	379.79	J/mol×K	757.06	Joback Method
cpg	387.01	J/mol×K	792.50	Joback Method
cpg	393.78	J/mol×K	827.93	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=R223997&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R223997&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>
<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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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