

# 1,2,3,4,7,8-Hexafluoro DBD

<b>Inchi:</b>	InChI=1S/C12H2F6O2/c13-3-1-5-6(2-4(3)14)20-12-10(18)8(16)7(15)9(17)11(12)19-5/h1-
<b>InchiKey:</b>	RCXWVRLURZAH RH-UHFFFAOYSA-N
<b>Formula:</b>	C12H2F6O2
<b>SMILES:</b>	Fc1cc2c(cc1F)Oc1c(F)c(F)c(F)c(F)c1O2
<b>Mol. weight [g/mol]:</b>	292.13

## Physical Properties

Property code	Value	Unit	Source
gf	-1062.60	kJ/mol	Joback Method
hf	-1251.07	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.419		Crippen Method
mvol	143.920	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
tb	623.82	K	Joback Method
tc	820.08	K	Joback Method
tf	460.38	K	Joback Method
vc	0.608	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.90	J/mol×K	623.82	Joback Method
cpg	367.20	J/mol×K	656.53	Joback Method
cpg	374.98	J/mol×K	689.24	Joback Method
cpg	382.29	J/mol×K	721.95	Joback Method
cpg	389.16	J/mol×K	754.66	Joback Method
cpg	395.61	J/mol×K	787.37	Joback Method
cpg	401.68	J/mol×K	820.08	Joback Method

# Sources

<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>
<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=R223942&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R223942&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>

# 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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