

# D-Arabinopyranose, tetrakis(trifluoroacetate) (isomer 2)

<b>Inchi:</b>	InChI=1S/C13H6F12O9/c14-10(15,16)6(26)31-2-1-30-5(34-9(29)13(23,24)25)4(33-8(28)
<b>InchiKey:</b>	ZHQMHGJNVQNHU-UHFFFAOYSA-N
<b>Formula:</b>	C13H6F12O9
<b>SMILES:</b>	O=C(OC1COC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	534.16

## Physical Properties

Property code	Value	Unit	Source
gf	-3288.26	kJ/mol	Joback Method
hf	-3817.87	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	70.18	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	1.871		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	1105.50		NIST Webbook
tb	812.81	K	Joback Method
tc	996.58	K	Joback Method
tf	562.90	K	Joback Method
vc	0.983	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.14	J/molxK	812.81	Joback Method
cpg	801.74	J/molxK	843.44	Joback Method
cpg	810.31	J/molxK	874.07	Joback Method
cpg	817.89	J/molxK	904.69	Joback Method
cpg	824.49	J/molxK	935.32	Joback Method
cpg	830.16	J/molxK	965.95	Joback Method
cpg	834.91	J/molxK	996.58	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=U380274&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380274&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.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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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