

# 1-O-(24-hyodeoxycholy)-«alpha»-D-glucopyranoside

**TFA**  
InchiKey:

InChI=1S/C42H44F18O15/c1-15(18-5-6-19-17-13-22(71-31(64)39(49,50)51)21-12-16(69

Formula:

C42H44F18O15

SMILES:

CC(CCC(=O)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=

Mol. weight [g/mol]:

1130.76

## Physical Properties

Property code	Value	Unit	Source
gf	-4786.20	kJ/mol	Joback Method
hf	-6181.43	kJ/mol	Joback Method
hfus	110.38	kJ/mol	Joback Method
hvap	150.68	kJ/mol	Joback Method
log10ws	-11.32		Crippen Method
logp	8.416		Crippen Method
mvol	638.150	ml/mol	McGowan Method
pc	402.90	kPa	Joback Method
rinpol	3323.00		NIST Webbook
rinpol	3323.00		NIST Webbook
tb	1714.69	K	Joback Method
tc	3031.07	K	Joback Method
tf	1176.11	K	Joback Method
vc	2.537	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3217.80	J/molxK	1714.69	Joback Method
cpg	3770.86	J/molxK	1934.09	Joback Method
cpg	4592.55	J/molxK	2153.48	Joback Method
cpg	5756.62	J/molxK	2372.88	Joback Method
cpg	7336.85	J/molxK	2592.27	Joback Method
cpg	9407.01	J/molxK	2811.67	Joback Method
cpg	12040.87	J/molxK	3031.07	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=R406563&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R406563&amp;Units=SI</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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