

# 1-O-(24-lithocholyl)-«beta»-D-glucopyranose, TFA

<b>Inchi:</b>	InChI=1S/C40H45F15O13/c1-16(20-7-8-21-19-6-5-17-14-18(63-30(58)37(44,45)46)10-1
<b>InchiKey:</b>	MCVCWLONWOKEQS-XUGJMOMDSA-N
<b>Formula:</b>	C40H45F15O13
<b>SMILES:</b>	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(=
<b>Mol. weight [g/mol]:</b>	1018.75

## Physical Properties

Property code	Value	Unit	Source
gf	-3979.82	kJ/mol	Joback Method
hf	-5277.93	kJ/mol	Joback Method
hfus	99.51	kJ/mol	Joback Method
hvap	141.12	kJ/mol	Joback Method
log10ws	-10.85		Crippen Method
logp	8.332		Crippen Method
mvol	597.220	ml/mol	McGowan Method
pc	455.21	kPa	Joback Method
rinsol	3404.00		NIST Webbook
tb	1602.73	K	Joback Method
tc	2452.50	K	Joback Method
tf	1081.46	K	Joback Method
vc	2.358	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2897.74	J/molxK	1602.73	Joback Method
cpg	3173.17	J/molxK	1744.36	Joback Method
cpg	3535.46	J/molxK	1885.99	Joback Method
cpg	4004.12	J/molxK	2027.61	Joback Method
cpg	4598.62	J/molxK	2169.24	Joback Method
cpg	5338.48	J/molxK	2310.87	Joback Method
cpg	6243.19	J/molxK	2452.50	Joback Method

# Sources

<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>
<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=R406607&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R406607&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>h vap:</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>m cvol:</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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