

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

Inchi:	InChI=1S/C40H45F15O13/c1-16(20-7-8-21-19-6-5-17-14-18(63-30(58)37(44,45)46)10-1
InchiKey:	MCVCWLONWOKEQS-OLJMSHAQSA-N
Formula:	C40H45F15O13
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]:	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
rinpol	3348.00		NIST Webbook
tb	1602.73	K	Joback Method
tc	2452.50	K	Joback Method
tf	1081.46	K	Joback Method
vc	2.358	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R406583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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