1-O-(24-cholyl)-«beta»-D-galactopyranose, TFA

Inchi: InChI=1S/C44H43F21O17/c1-14(4-7-23(66)79-28-27(82-35(73)44(63,64)65)26(81-34(72

InchiKey: QHOCKXCFQMXQIH-XNAUKSFJSA-N

Formula: C44H43F21O17

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]: 1242.77

Physical Properties

Property code	Value	Unit	Source
gf	-5592.58	kJ/mol	Joback Method
hf	-7084.93	kJ/mol	Joback Method
hfus	121.24	kJ/mol	Joback Method
hvap	160.23	kJ/mol	Joback Method
log10ws	-11.80		Crippen Method
logp	8.500		Crippen Method
mcvol	679.080	ml/mol	McGowan Method
pc	359.11	kPa	Joback Method
rinpol	3328.00		NIST Webbook
tb	1826.65	K	Joback Method
tc	3978.91	K	Joback Method
tf	1270.76	K	Joback Method
vc	2.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3570.24	J/mol×K	1826.65	Joback Method
cpg	4802.22	J/mol×K	2185.36	Joback Method
cpg	6975.41	J/mol×K	2544.07	Joback Method
cpg	10417.89	J/mol×K	2902.78	Joback Method
cpg	15457.75	J/mol×K	3261.49	Joback Method
cpg	22423.06	J/mol×K	3620.20	Joback Method
cpg	31641.93	J/mol×K	3978.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R406518&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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

Latest version available from:
https://www.chemeo.com/cid/19-727-4/1-O-24-cholyl-beta-D-galactopyranose-TFA.pdf
Generated by Cheméo on 2024-04-24 04:19:58.473193978 +0000 UTC m=+16221647.393771289.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.