1-O-(24-chenodeoxycholyl)-«beta»-D-glucopyranc TFA

InChI: InChI=1S/C42H44F18O15/c1-15(18-5-6-19-24-20(9-11-36(18,19)3)35(2)10-8-17(69-30(6
InchiKey: YGPQRMKMRCMANY-YXTYLQBASA-N
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
mcvol	638.150	ml/mol	McGowan Method
pc	402.90	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1714.69	K	Joback Method
tc	3031.07	K	Joback Method
tf	1176.11	K	Joback Method
vc	2.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3217.80	J/mol×K	1714.69	Joback Method
cpg	3770.86	J/mol×K	1934.09	Joback Method
cpg	4592.55	J/mol×K	2153.48	Joback Method
cpg	5756.62	J/mol×K	2372.88	Joback Method
cpg	7336.85	J/mol×K	2592.27	Joback Method
cpg	9407.01	J/mol×K	2811.67	Joback Method
cpg	12040.87	J/mol×K	3031.07	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=R406494&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
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