Etiocholan-3«alpha»-ol-17-one, trifluoroacetate

Inchi: InChI=1S/C21H29F3O3/c1-19-9-7-13(27-18(26)21(22,23)24)11-12(19)3-4-14-15-5-6-17(

InchiKey: NTPCFTHVUCOBOX-UHFFFAOYSA-N

Formula: C21H29F3O3

SMILES: CC12CCC3C(CCC4CC(OC(=O)C(F)(F)F)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 386.45

Physical Properties

Property code	Value	Unit	Source
hfus	26.93	kJ/mol	Joback Method
log10ws	-5.33		Cheméo Relay (1.0)
logp	5.072		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
rinpol	2431.70		NIST Webbook
tf	412.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.23	J/mol×K	853.35	Joback Method
cpg	1024.27	J/mol×K	891.77	Joback Method
cpg	1049.07	J/mol×K	930.19	Joback Method
cpg	1073.95	J/mol×K	968.60	Joback Method
cpg	1099.21	J/mol×K	1007.02	Joback Method
cpg	1125.16	J/mol×K	1045.44	Joback Method
cpg	1152.12	J/mol×K	1083.86	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352247&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point