PROPRANOLOL BIS(TRIFLUOROACETATE)

Other names: Propranolol, bis-TFA
propranolol, TFA
Inchi: InChI=1S/C20H19F6NO4/c1-12(2)27(17(28)19(21,22)23)10-14(31-18(29)20(24,25)26)11
InchiKey: QALUHRIUDJFKPS-UHFFFAOYSA-N
Formula: C20H19F6NO4
SMILES: CC(C)N(CC(COc1cccc2ccccc12)OC(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]: 451.36

Physical Properties

Property code	Value	Unit	Source
hfus	43.43	kJ/mol	Joback Method
log10ws	-4.83		Cheméo Relay (1.0)
logp	4.492		Crippen Method
mcvol	284.920	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.73	J/mol×K	860.94	Joback Method
cpg	904.28	J/mol×K	894.40	Joback Method
cpg	915.91	J/mol×K	927.87	Joback Method
cpg	926.72	J/mol×K	961.33	Joback Method
cpg	936.79	J/mol×K	994.79	Joback Method
cpg	946.22	J/mol×K	1028.26	Joback Method
cpg	955.09	J/mol×K	1061.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40435878&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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