Alprenolol, N,O-di(trifluoroacetyl)-

Inchi: InChI=1S/C19H21F6NO4/c1-4-7-13-8-5-6-9-15(13)29-11-14(30-17(28)19(23,24)25)10-26
InchiKey: CFMTYXOXDDMWHX-UHFFFAOYSA-N
Formula: C19H21F6NO4
SMILES: C=CCc1ccccc1OCC(CN(C(=O)C(F)(F)F)C(C)C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 441.37

Physical Properties

Property code	Value	Unit	Source
hfus	42.54	kJ/mol	Joback Method
log10ws	-4.26		Cheméo Relay (1.0)
logp	4.067		Crippen Method
mcvol	285.990	ml/mol	McGowan Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tf	314.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.66	J/mol×K	815.76	Joback Method
cpg	896.19	J/mol×K	847.34	Joback Method
cpg	908.75	J/mol×K	878.91	Joback Method
cpg	920.39	J/mol×K	910.49	Joback Method
cpg	931.19	J/mol×K	942.07	Joback Method
cpg	941.20	J/mol×K	973.65	Joback Method
cpg	950.47	J/mol×K	1005.22	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40435856&Units=SI

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