Oxprenolol, TFA

Inchi: InChI=1S/C19H21F6NO5/c1-4-9-29-13-5-7-14(8-6-13)30-11-15(31-17(28)19(23,24)25)10
InchiKey: YRNQUNDGDDKMQD-UHFFFAOYSA-N
Formula: C19H21F6NO5
SMILES: C=CCOc1ccc(OCC(CN(C(=O)C(F)(F)F)C(C)C)OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 457.36

Physical Properties

Property code	Value	Unit	Source
gf	-1330.40	kJ/mol	Joback Method
hf	-1844.01	kJ/mol	Joback Method
hfus	43.73	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.904		Crippen Method
mcvol	291.860	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	1930.00		NIST Webbook
tb	838.18	K	Joback Method
tc	1030.11	K	Joback Method
tf	518.47	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.61	J/mol×K	838.18	Joback Method
cpg	923.81	J/mol×K	870.17	Joback Method
cpg	935.99	J/mol×K	902.16	Joback Method
cpg	947.21	J/mol×K	934.14	Joback Method
cpg	957.51	J/mol×K	966.13	Joback Method
cpg	966.95	J/mol×K	998.12	Joback Method
cpg	975.58	J/mol×K	1030.11	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=R314206&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