

Toliprolol, HFB

Inchi:	InChI=1S/C21H19F14NO4/c1-10(2)36(14(37)16(22,23)18(26,27)20(30,31)32)8-13(9-39-
InchiKey:	WZLIKHISFPDOOW-UHFFFAOYSA-N
Formula:	C21H19F14NO4
SMILES:	Cc1cccc(OCC(CN(C(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(C)C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F)
Mol. weight [g/mol]:	615.36

Physical Properties

Property code	Value	Unit	Source
gf	-2843.52	kJ/mol	Joback Method
hf	-3482.38	kJ/mol	Joback Method
hfus	43.98	kJ/mol	Joback Method
hvap	65.64	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.188		Crippen Method
mcvol	332.630	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinqol	1748.00		NIST Webbook
tb	846.08	K	Joback Method
tc	1036.08	K	Joback Method
tf	534.94	K	Joback Method
vc	1.343	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.84	J/molxK	846.08	Joback Method
cpg	1101.60	J/molxK	877.75	Joback Method
cpg	1113.41	J/molxK	909.41	Joback Method
cpg	1124.41	J/molxK	941.08	Joback Method
cpg	1134.71	J/molxK	972.75	Joback Method
cpg	1144.44	J/molxK	1004.42	Joback Method
cpg	1153.73	J/molxK	1036.08	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=R314231&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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