

Toliprolol, TFA

Inchi: InChI=1S/C17H19F6NO4/c1-10(2)24(14(25)16(18,19)20)8-13(28-15(26)17(21,22)23)9-2
InchiKey: RKNLDVQEQLJGFY-UHFFFAOYSA-N
Formula: C17H19F6NO4
SMILES: Cc1cccc(OCC(CN(C(=O)C(F)(F)F)C(C)C)OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 415.33

Physical Properties

Property code	Value	Unit	Source
gf	-1330.08	kJ/mol	Joback Method
hf	-1795.94	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.647		Crippen Method
mcvol	262.110	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinqol	1728.00		NIST Webbook
tb	773.32	K	Joback Method
tc	958.90	K	Joback Method
tf	475.46	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.90	J/molxK	773.32	Joback Method
cpg	809.33	J/molxK	804.25	Joback Method
cpg	821.80	J/molxK	835.18	Joback Method
cpg	833.38	J/molxK	866.11	Joback Method
cpg	844.11	J/molxK	897.04	Joback Method
cpg	854.03	J/molxK	927.97	Joback Method
cpg	863.20	J/molxK	958.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R314246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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