

Exaprolol, TFA

Inchi:	InChI=1S/C20H28F3NO3/c1-14(2)24(19(26)20(21,22)23)12-16(25)13-27-18-11-7-6-10-1
InchiKey:	XDDFLIVZVSWUMO-UHFFFAOYSA-N
Formula:	C20H28F3NO3
SMILES:	CC(C)N(CC(O)COc1cccc1C1CCCC1)C(=O)C(F)(F)F
Mol. weight [g/mol]:	387.44

Physical Properties

Property code	Value	Unit	Source
gf	-601.68	kJ/mol	Joback Method
hf	-1113.89	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.273		Crippen Method
mvol	286.640	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
tb	882.82	K	Joback Method
tc	1088.17	K	Joback Method
tf	501.12	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.12	J/molxK	882.82	Joback Method
cpg	970.38	J/molxK	917.05	Joback Method
cpg	984.47	J/molxK	951.27	Joback Method
cpg	997.45	J/molxK	985.50	Joback Method
cpg	1009.40	J/molxK	1019.72	Joback Method
cpg	1020.39	J/molxK	1053.95	Joback Method
cpg	1030.51	J/molxK	1088.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=R217888&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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