Exaprolol, HFB

Inchi: InChI=1S/C22H28F7NO3/c1-14(2)30(19(32)20(23,24)21(25,26)22(27,28)29)12-16(31)13
InchiKey: OQLCBAGSZKDZJS-UHFFFAOYSA-N
Formula: C22H28F7NO3
SMILES: CC(C)N(CC(O)COc1ccccc1C1CCCCC1)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 487.45

Physical Properties

Property code	Value	Unit	Source
gf	-1358.40	kJ/mol	Joback Method
hf	-1957.11	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.544		Crippen Method
mcvol	321.900	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2160.00		NIST Webbook
tb	919.20	K	Joback Method
tc	1125.73	K	Joback Method
tf	530.86	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.10	J/mol×K	919.20	Joback Method
cpg	1118.83	J/mol×K	953.62	Joback Method
cpg	1132.51	J/mol×K	988.04	Joback Method
cpg	1145.25	J/mol×K	1022.47	Joback Method
cpg	1157.20	J/mol×K	1056.89	Joback Method
cpg	1168.45	J/mol×K	1091.31	Joback Method
cpg	1179.15	J/mol×K	1125.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R217873&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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