

propranolol, HFB

Inchi:	InChI=1S/C24H19F14NO4/c1-12(2)39(17(40)19(25,26)21(29,30)23(33,34)35)10-14(43-1
InchiKey:	XBHHNHGLKQIVNW-UHFFFAOYSA-N
Formula:	C24H19F14NO4
SMILES:	CC(C)N(CC(COC1CCCC2CCCCC12)OC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(=O)C(F)(F)C(F)(F)C(F)(F)C
Mol. weight [g/mol]:	651.39

Physical Properties

Property code	Value	Unit	Source
gf	-2711.61	kJ/mol	Joback Method
hf	-3353.23	kJ/mol	Joback Method
hfus	48.77	kJ/mol	Joback Method
hvap	73.96	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	7.033		Crippen Method
mcvol	355.440	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinsol	2133.00		NIST Webbook
tb	933.70	K	Joback Method
tc	1145.21	K	Joback Method
tf	601.45	K	Joback Method
vc	1.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1183.98	J/molxK	933.70	Joback Method
cpg	1196.55	J/molxK	968.95	Joback Method
cpg	1208.50	J/molxK	1004.20	Joback Method
cpg	1220.03	J/molxK	1039.46	Joback Method
cpg	1231.34	J/molxK	1074.71	Joback Method
cpg	1242.65	J/molxK	1109.96	Joback Method
cpg	1254.14	J/molxK	1145.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R314211&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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