

Bupranolol, hydroxy, acetylated

Inchi:	InChI=1S/C20H28ClNO6/c1-12-8-19(17(21)9-18(12)28-15(4)25)26-11-16(27-14(3)24)10
InchiKey:	JLOBLUPBRPXJKV-UHFFFAOYSA-N
Formula:	C20H28ClNO6
SMILES:	CC(=O)Oc1cc(Cl)c(OCC(CN(C(C)=O)C(C)(C)C)OC(C)=O)cc1C
Mol. weight [g/mol]:	413.89

Physical Properties

Property code	Value	Unit	Source
gf	-401.47	kJ/mol	Joback Method
hf	-950.65	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	96.59	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.531		Crippen Method
mcvol	313.440	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	2260.00		NIST Webbook
tb	973.69	K	Joback Method
tc	1196.91	K	Joback Method
tf	645.43	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.58	J/molxK	973.69	Joback Method
cpg	997.80	J/molxK	1010.89	Joback Method
cpg	1008.63	J/molxK	1048.10	Joback Method
cpg	1018.13	J/molxK	1085.30	Joback Method
cpg	1026.30	J/molxK	1122.51	Joback Method
cpg	1033.20	J/molxK	1159.71	Joback Method
cpg	1038.84	J/molxK	1196.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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