

Metipranolol, desamino hydroxy, acetylated

Inchi:	InChI=1S/C18H24O7/c1-10-7-17(11(2)12(3)18(10)25-15(6)21)23-9-16(24-14(5)20)8-22-
InchiKey:	GCUVLNNO DRMMBF-UHFFFAOYSA-N
Formula:	C18H24O7
SMILES:	CC(=O)OCC(COc1cc(C)c(OC(C)=O)c(C)c1C)OC(C)=O
Mol. weight [g/mol]:	352.38

Physical Properties

Property code	Value	Unit	Source
gf	-634.63	kJ/mol	Joback Method
hf	-1096.10	kJ/mol	Joback Method
hfus	40.89	kJ/mol	Joback Method
hvap	90.08	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.411		Crippen Method
mvol	268.910	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	908.69	K	Joback Method
tc	1121.91	K	Joback Method
tf	592.83	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.58	J/molxK	908.69	Joback Method
cpg	842.08	J/molxK	944.23	Joback Method
cpg	853.19	J/molxK	979.76	Joback Method
cpg	862.86	J/molxK	1015.30	Joback Method
cpg	871.06	J/molxK	1050.84	Joback Method
cpg	877.76	J/molxK	1086.37	Joback Method
cpg	882.94	J/molxK	1121.91	Joback Method
dvisc	0.0002313	Paxs	592.83	Joback Method
dvisc	0.0001510	Paxs	645.47	Joback Method

dvisc	0.0001052	Paxs	698.12	Joback Method
dvisc	0.0000770	Paxs	750.76	Joback Method
dvisc	0.0000588	Paxs	803.40	Joback Method
dvisc	0.0000464	Paxs	856.05	Joback Method
dvisc	0.0000376	Paxs	908.69	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=R582726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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