

Alprenolol desaminodihydroxy, acetylated

Inchi:	InChI=1S/C18H22O7/c1-5-6-15-9-16(24-13(3)20)7-8-18(15)23-11-17(25-14(4)21)10-22-
InchiKey:	UGLDVYYRPLVKDT-UHFFFAOYSA-N
Formula:	C18H22O7
SMILES:	<chem>C=CCc1cc(OC(C)=O)ccc1OCC(COC(C)=O)OC(C)=O</chem>
Mol. weight [g/mol]:	350.36

Physical Properties

Property code	Value	Unit	Source
gf	-527.53	kJ/mol	Joback Method
hf	-947.73	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	88.08	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.214		Crippen Method
mvol	264.610	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
tb	895.41	K	Joback Method
tc	1108.27	K	Joback Method
tf	566.03	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/molxK	895.41	Joback Method
cpg	816.24	J/molxK	930.89	Joback Method
cpg	827.24	J/molxK	966.36	Joback Method
cpg	836.91	J/molxK	1001.84	Joback Method
cpg	845.25	J/molxK	1037.32	Joback Method
cpg	852.24	J/molxK	1072.80	Joback Method
cpg	857.86	J/molxK	1108.27	Joback Method
dvisc	0.0002990	Paxs	566.03	Joback Method

dvisc	0.0001832	Paxs	620.93	Joback Method
dvisc	0.0001216	Paxs	675.82	Joback Method
dvisc	0.0000858	Paxs	730.72	Joback Method
dvisc	0.0000636	Paxs	785.62	Joback Method
dvisc	0.0000490	Paxs	840.51	Joback Method
dvisc	0.0000390	Paxs	895.41	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=R582424&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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