1,2-Diacetoxy-3-[4-acetoxy-2-(2-acetoxy)propyl]ph

Other names: Alprenolol desaminodihydroxy + H2O, acetylated
Inchi: InChI=1S/C20H26O9/c1-12(27-14(3)22)8-17-9-18(28-15(4)23)6-7-20(17)26-11-19(29-16
InchiKey: XCGBFJXUDBUTAP-UHFFFAOYSA-N
Formula: C20H26O9
SMILES: CC(=O)OCC(COc1ccc(OC(C)=O)cc1CC(C)OC(C)=O)OC(C)=O
Mol. weight [g/mol]: 410.42

Physical Properties

Property code	Value	Unit	Source
gf	-834.89	kJ/mol	Joback Method
hf	-1364.52	kJ/mol	Joback Method
hfus	46.11	kJ/mol	Joback Method
hvap	101.97	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	1.980		Crippen Method
mcvol	304.530	ml/mol	McGowan Method
pc	1419.71	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	1020.34	K	Joback Method
tc	1249.73	K	Joback Method
tf	647.49	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.77	J/mol×K	1020.34	Joback Method
cpg	1006.37	J/mol×K	1211.50	Joback Method
cpg	1005.59	J/mol×K	1173.27	Joback Method
cpg	1002.71	J/mol×K	1135.04	Joback Method
cpg	997.75	J/mol×K	1096.80	Joback Method
cpg	990.76	J/mol×K	1058.57	Joback Method
cpg	1005.01	J/mol×K	1249.73	Joback Method

dvisc	0.0000170	Pa×s	1020.34	Joback Method
dvisc	0.0000216	Pa×s	958.20	Joback Method
dvisc	0.0000285	Pa×s	896.06	Joback Method
dvisc	0.0000390	Pa×s	833.91	Joback Method
dvisc	0.0000563	Pa×s	771.77	Joback Method
dvisc	0.0000866	Pa×s	709.63	Joback Method
dvisc	0.0001447	Pa×s	647.49	Joback Method

Sources

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=U281341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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