1-(2,3-Diacetoxypropoxy)-2-(2-acetoxypropyl)benz

Other names: Alprenolol desaminohydroxy + H2O, acetylated
Inchi: InChI=1S/C18H24O7/c1-12(24-14(3)20)9-16-7-5-6-8-18(16)23-11-17(25-15(4)21)10-22-1
InchiKey: OUGIXDAAJGZKRM-UHFFFAOYSA-N
Formula: C18H24O7
SMILES: CC(=O)OCC(COc1ccccc1CC(C)OC(C)=O)OC(C)=O
Mol. weight [g/mol]: 352.38

Physical Properties

Property code	Value	Unit	Source
gf	-608.18	kJ/mol	Joback Method
hf	-1066.97	kJ/mol	Joback Method
hfus	38.53	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.054		Crippen Method
mcvol	268.910	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	893.31	K	Joback Method
tc	1105.62	K	Joback Method
tf	540.27	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.70	J/mol×K	893.31	Joback Method
cpg	884.57	J/mol×K	1070.24	Joback Method
cpg	877.18	J/mol×K	1034.85	Joback Method
cpg	868.39	J/mol×K	999.47	Joback Method
cpg	858.20	J/mol×K	964.08	Joback Method
cpg	846.64	J/mol×K	928.70	Joback Method
cpg	890.53	J/mol×K	1105.62	Joback Method

dvisc	0.0000326	Pa×s	893.31	Joback Method
dvisc	0.0000423	Pa×s	834.47	Joback Method
dvisc	0.0000570	Pa×s	775.63	Joback Method
dvisc	0.0000807	Pa×s	716.79	Joback Method
dvisc	0.0001217	Pa×s	657.95	Joback Method
dvisc	0.0001989	Pa×s	599.11	Joback Method
dvisc	0.0003617	Pa×s	540.27	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=U280763&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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