1,6-Anhydro-2,3-O-isopropylidene-«beta»-D-mann

Inchi: InChI=1S/C9H14O5/c1-9(2)13-6-5(10)4-3-11-8(12-4)7(6)14-9/h4-8,10H,3H2,1-2H3
InchiKey: VEESJHGZLRXGHP-UHFFFAOYSA-N
Formula: C9H14O5
SMILES: CC1(C)OC2C3OCC(O3)C(O)C2O1
Mol. weight [g/mol]: 202.20
CAS: 14440-51-8

Physical Properties

Property code	Value	Unit	Source
gf	-326.97	kJ/mol	Joback Method
hf	-749.02	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	-0.378		Crippen Method
mcvol	134.440	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	1436.60		NIST Webbook
tb	620.29	K	Joback Method
tc	831.31	K	Joback Method
tf	416.25	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.87	J/mol×K	620.29	Joback Method
cpg	433.31	J/mol×K	655.46	Joback Method
cpg	446.90	J/mol×K	690.63	Joback Method
cpg	459.76	J/mol×K	725.80	Joback Method
cpg	472.03	J/mol×K	760.97	Joback Method
cpg	483.85	J/mol×K	796.14	Joback Method
cpg	495.36	J/mol×K	831.31	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=C14440518&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
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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