Riesling acetal

Inchi: InChI=1S/C12H18O2/c1-10(2)6-4-7-11(3)12(10)8-5-9(13-11)14-12/h4,7,9H,5-6,8H2,1-3H
InchiKey: DFJRLXSMMWWPFG-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CC1(C)CC=CC2(C)OC3CCC12O3
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	41.75	kJ/mol	Joback Method
hf	-265.77	kJ/mol	Joback Method
hfus	16.40	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.637		Crippen Method
mcvol	154.800	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
ripol	1637.00		NIST Webbook
ripol	1656.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1612.00		NIST Webbook
ripol	1637.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1637.00		NIST Webbook
tb	551.83	K	Joback Method
tc	794.31	K	Joback Method
tf	393.14	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.84	J/mol×K	551.83	Joback Method
cpg	437.14	J/mol×K	592.24	Joback Method

cpg	454.71	J/mol×K	632.66	Joback Method
cpg	471.05	J/mol×K	673.07	Joback Method
cpg	486.63	J/mol×K	713.49	Joback Method
cpg	501.95	J/mol×K	753.90	Joback Method
cpg	517.48	J/mol×K	794.31	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=R302728&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume