(4aR,5S)-1-Hydroxy-4a,5-dimethyl-3-(propan-2-yli

Inchi: InChI=1S/C15H22O2/c1-9(2)11-8-15(4)10(3)6-5-7-12(15)14(17)13(11)16/h10,17H,5-8H2
InchiKey: PIGIXBXGOOKXOZ-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC(C)=C1CC2(C)C(=C(O)C1=O)CCCC2C
Mol. weight [g/mol]: 234.33
CAS: 4895-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-68.77	kJ/mol	Joback Method
hf	-405.58	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	71.76	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.934		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	749.04	K	Joback Method
tc	970.75	K	Joback Method
tf	455.75	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.91	J/mol×K	749.04	Joback Method
cpg	621.44	J/mol×K	785.99	Joback Method
cpg	638.29	J/mol×K	822.94	Joback Method
cpg	654.57	J/mol×K	859.90	Joback Method
cpg	670.41	J/mol×K	896.85	Joback Method
cpg	685.92	J/mol×K	933.80	Joback Method
cpg	701.23	J/mol×K	970.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4895425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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