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

Inchi: InChI=1S/C15H20O2/c1-9(2)11-8-15(4)10(3)6-5-7-12(15)14(17)13(11)16/h5,7,10,17H,6,8

InchiKey: IRTXMQLWUFCOHH-UHFFFAOYSA-N

Formula: C15H20O2

SMILES: CC(C)=C1CC2(C)C(=C(O)C1=O)C=CCC2C

Mol. weight [g/mol]: 232.32

CAS: 669064-29-3

Physical Properties

Property code	Value	Unit	Source
gf	-38.81	kJ/mol	Joback Method
hf	-347.80	kJ/mol	Joback Method
hfus	20.46	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.710		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1895.10		NIST Webbook
rinpol	1895.10		NIST Webbook
tb	748.20	K	Joback Method
tc	971.61	K	Joback Method
tf	456.51	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.26	J/mol×K	748.20	Joback Method
cpg	594.86	J/mol×K	785.43	Joback Method
cpg	610.82	J/mol×K	822.67	Joback Method
cpg	626.27	J/mol×K	859.90	Joback Method
cpg	641.34	J/mol×K	897.14	Joback Method
cpg	656.14	J/mol×K	934.37	Joback Method
cpg	670.81	J/mol×K	971.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C669064293&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