(2R,3R,4aR,5S)-2-Hydroxy-4a,5-dimethyl-3-(prop-1

Inchi: InChI=1S/C15H22O2/c1-9(2)11-8-15(4)10(3)6-5-7-12(15)14(17)13(11)16/h7,10-11,13,16
InchiKey: XFRADCOKSLIXIG-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C(C)C1CC2(C)C(=CCCC2C)C(=O)C1O
Mol. weight [g/mol]: 234.33
CAS: 5090-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-32.18	kJ/mol	Joback Method
hf	-385.39	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.875		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1864.20		NIST Webbook
rinpol	1864.20		NIST Webbook
tb	724.76	K	Joback Method
tc	943.96	K	Joback Method
tf	422.63	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.52	J/mol×K	724.76	Joback Method
cpg	629.22	J/mol×K	761.29	Joback Method
cpg	647.05	J/mol×K	797.83	Joback Method
cpg	664.12	J/mol×K	834.36	Joback Method
cpg	680.55	J/mol×K	870.89	Joback Method
cpg	696.45	J/mol×K	907.43	Joback Method
cpg	711.93	J/mol×K	943.96	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C5090904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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