(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethyl-3-(pr

Inchi: InChI=1S/C15H22O2/c1-9(2)11-8-15(4)10(3)6-5-7-12(15)14(17)13(11)16/h5,7,10-13,16H
InchiKey: UALVHXGADCCBEW-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C(C)C1CC2(C)C(C)CC=CC2C(=O)C1O
Mol. weight [g/mol]: 234.33
CAS: 5090-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-30.26	kJ/mol	Joback Method
hf	-394.26	kJ/mol	Joback Method
hfus	21.62	kJ/mol	Joback Method
hvap	68.05	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.731		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	1776.50		NIST Webbook
rinpol	1776.50		NIST Webbook
tb	715.11	K	Joback Method
tc	933.51	K	Joback Method
tf	405.87	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.50	J/mol×K	715.11	Joback Method
cpg	632.77	J/mol×K	751.51	Joback Method
cpg	651.09	J/mol×K	787.91	Joback Method
cpg	668.58	J/mol×K	824.31	Joback Method
cpg	685.35	J/mol×K	860.71	Joback Method
cpg	701.50	J/mol×K	897.11	Joback Method
cpg	717.16	J/mol×K	933.51	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=C5090891&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