7-epi-bourbon-3-en-5,11-oxide

Inchi: InChI=1S/C15H22O/c1-9-5-6-11-14(4)8-7-10-12(14)15(9,11)16-13(10,2)3/h5,10-12H,6-8
InchiKey: MMJLGRDTAHXVGD-ZCRGAIPPSA-N
Formula: C15H22O
SMILES: CC1=CCC2C3(C)CCC4C3C12OC4(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	220.74	kJ/mol	Joback Method
hf	-142.38	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.546		Crippen Method
mcvol	180.340	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1471.00		NIST Webbook
tb	592.03	K	Joback Method
tc	824.75	K	Joback Method
tf	433.64	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.88	J/mol×K	592.03	Joback Method
cpg	540.32	J/mol×K	630.82	Joback Method
cpg	559.35	J/mol×K	669.60	Joback Method
cpg	577.46	J/mol×K	708.39	Joback Method
cpg	595.11	J/mol×K	747.17	Joback Method
cpg	612.80	J/mol×K	785.96	Joback Method
cpg	630.99	J/mol×K	824.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407680&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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