2-epi-Ziza-6(13)-en-3-one

Other names: 2-epi-Ziza-6(13)-en-3-one (methyl group in 2-«alpha»-position)
Inchi: InChI=1S/C15H22O/c1-9-12-7-13(16)10(2)15(12)6-5-11(8-15)14(9,3)4/h10-12H,1,5-8H2,
InchiKey: RVQOGXCBZWSGSS-SBXIWPSPSA-N
Formula: C15H22O
SMILES: C=C1C2CC(=O)C(C)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	137.56	kJ/mol	Joback Method
hf	-210.51	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	50.55	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1660.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2295.00		NIST Webbook
tb	629.48	K	Joback Method
tc	866.95	K	Joback Method
tf	426.81	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.93	J/mol×K	629.48	Joback Method
cpg	563.88	J/mol×K	669.06	Joback Method
cpg	584.68	J/mol×K	708.64	Joback Method
cpg	604.63	J/mol×K	748.22	Joback Method
cpg	624.03	J/mol×K	787.79	Joback Method

cpg	643.18	J/mol×K	827.37	Joback Method
cpg	662.38	J/mol×K	866.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198737&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume