(+)-Barbatenal

Inchi: InChI=1S/C15H22O/c1-13-8-5-11(10-16)12(9-13)14(2)6-4-7-15(13,14)3/h5,10,12H,4,6-9
InchiKey: GVADVPQNXLRSBB-DKUMPPAJSA-N
Formula: C15H22O
SMILES: CC12CC=C(C=O)C(C1)C1(C)CCCC21C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	130.10	kJ/mol	Joback Method
hf	-160.74	kJ/mol	Joback Method
hfus	10.11	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
tb	620.21	K	Joback Method
tc	856.90	K	Joback Method
tf	428.33	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.78	J/mol×K	620.21	Joback Method
cpg	546.55	J/mol×K	659.66	Joback Method
cpg	565.25	J/mol×K	699.11	Joback Method
cpg	583.33	J/mol×K	738.56	Joback Method
cpg	601.25	J/mol×K	778.01	Joback Method
cpg	619.48	J/mol×K	817.45	Joback Method
cpg	638.48	J/mol×K	856.90	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=R515687&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume