«alpha»-Barbatenal

Inchi: InChI=1S/C16H24/c1-5-12-7-10-14(2)11-13(12)15(3)8-6-9-16(14,15)4/h5,7,13H,1,6,8-11
InchiKey: OGCDVJZYJHNLRC-JONQDZQNSA-N
Formula: C16H24
SMILES: C=CC1=CCC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]: 216.36

Physical Properties

Property code	Value	Unit	Source
gf	325.88	kJ/mol	Joback Method
hf	29.63	kJ/mol	Joback Method
hfus	9.13	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.725		Crippen Method
mcvol	195.120	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1707.00		NIST Webbook
rinpol	1707.00		NIST Webbook
tb	591.11	K	Joback Method
tc	826.45	K	Joback Method
tf	395.84	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.38	J/mol×K	591.11	Joback Method
cpg	554.40	J/mol×K	630.33	Joback Method
cpg	574.95	J/mol×K	669.56	Joback Method
cpg	594.48	J/mol×K	708.78	Joback Method
cpg	613.47	J/mol×K	748.01	Joback Method
cpg	632.36	J/mol×K	787.23	Joback Method
cpg	651.64	J/mol×K	826.45	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=R424289&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