4,5-di-epi-aristolochene

Inchi: InChI=1S/C15H24/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h9,12-13H,1,5-8,10H2,2-
InchiKey: YONHOSLUBQJXPR-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C(C)C1CC=C2CCCC(C)C2(C)C1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	234.94	kJ/mol	Joback Method
hf	-75.12	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
tb	569.43	K	Joback Method
tc	794.31	K	Joback Method
tf	297.83	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/mol×K	569.43	Joback Method
cpg	523.17	J/mol×K	606.91	Joback Method
cpg	545.19	J/mol×K	644.39	Joback Method
cpg	565.88	J/mol×K	681.87	Joback Method
cpg	585.40	J/mol×K	719.35	Joback Method
cpg	603.90	J/mol×K	756.83	Joback Method
cpg	621.57	J/mol×K	794.31	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=U374171&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

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