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-JHIQODARSA-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
hfus	15.49	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Cheméo Relay (1.0)
ie	8.22	eV	Cheméo Relay (1.0)
log10ws	-5.37		Cheméo Relay (1.0)
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1469.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1665.00		NIST Webbook
tb	543.69	K	Cheméo Relay (1.0)
tf	292.93	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241326&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point