

ent-(+)-Amorpha-4,11-diene

Inchi: InChI=1S/C15H24/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h9,12,14-15H,5-8H2,1-4H
InchiKey: YBEONGKDMARZSS-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CC2C(=C(C)C)CCC(C)C2CC1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	198.05	kJ/mol	Joback Method
hf	-139.76	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
tb	579.15	K	Joback Method
tc	797.50	K	Joback Method
tf	286.05	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.43	J/mol×K	579.15	Joback Method
cpg	526.45	J/mol×K	615.54	Joback Method
cpg	548.11	J/mol×K	651.93	Joback Method
cpg	568.46	J/mol×K	688.33	Joback Method
cpg	587.58	J/mol×K	724.72	Joback Method
cpg	605.50	J/mol×K	761.11	Joback Method
cpg	622.30	J/mol×K	797.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R303043&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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