

5(-)-Gymnomitr-3(15)-4-diene

Inchi:	InChI=1S/C15H22/c1-11-6-9-13(2)10-12(11)14(3)7-5-8-15(13,14)4/h6,9,12H,1,5,7-8,10H
InchiKey:	JRVADZCIHISZKL-DKUMPPAJSA-N
Formula:	C15H22
SMILES:	C=C1C=CC2(C)CC1C1(C)CCCC21C
Mol. weight [g/mol]:	202.34

Physical Properties

Property code	Value	Unit	Source
gf	292.33	kJ/mol	Joback Method
hf	20.55	kJ/mol	Joback Method
hfus	7.05	kJ/mol	Joback Method
hvap	45.76	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook
tb	565.73	K	Joback Method
tc	801.71	K	Joback Method
tf	387.49	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.56	J/molxK	565.73	Joback Method
cpg	501.99	J/molxK	605.06	Joback Method
cpg	521.76	J/molxK	644.39	Joback Method
cpg	540.33	J/molxK	683.72	Joback Method
cpg	558.16	J/molxK	723.05	Joback Method
cpg	575.70	J/molxK	762.38	Joback Method
cpg	593.40	J/molxK	801.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R515761&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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