cis-Thujopsene

Other names:	Thujopsene
	Cyclopropa[d]naphthalene, 1,1a,4,4a,5,6,7,8-octahydro-2,4a,8,8-tetramethyl-, [1aS-(1a«alpha»,4a«beta»,8aR*)]-
	Cyclopropa[d]naphthalene, 1,1a,4,4a,5,6,7,8-octahydro-2,4a,8,8-tetramethyl-, (1aS,4aS,8aS)-(-)-
	Sesquichamene
	Thujopsen
	Widdrene
	cis-(-)-Thujopsene
	(Z)-Thujopsene
	[1aS-(1a«alpha»,4a«beta»,8aR*)]-1,1a,4,4a,5,6,7,8-octahydro-2,4a,8,8-tetramethylcyclop
Inchi:	InChI=1S/C15H24/c1-11-6-9-14(4)8-5-7-13(2,3)15(14)10-12(11)15/h6,12H,5,7-10H2,1-4
InchiKey:	WXQGPFZDVCRBME-BLZCZZARSA-N
Formula:	C15H24
SMILES:	CC1=CCC2(C)CCCC(C)(C)C23CC13
Mol. weight [g/mol]:	204.35
CAS:	470-40-6

Physical Properties

Property code	Value	Unit	Source
gf	229.62	kJ/mol	Joback Method
hf	-75.16	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1426.00		NIST Webbook
rinpol	1431.00		NIST Webbook

rinpol	1441.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1431.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1425.00	NIST Webbook
rinpol	1430.00	NIST Webbook
rinpol	1441.00	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1446.80	NIST Webbook
rinpol	1430.50	NIST Webbook
rinpol	1431.00	NIST Webbook
rinpol	1429.00	NIST Webbook
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rinpol	1441.50	NIST Webbook
rinpol	1456.00	NIST Webbook
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rinpol	1441.00	NIST Webbook
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rinpol	1429.00	NIST Webbook
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rinpol	1416.00	NIST Webbook
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rinpol	1432.00	NIST Webbook
rinpol	1435.00	NIST Webbook
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rinpol	1438.00		NIST Webbook
rinpol	1450.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1660.00		NIST Webbook
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ripol	1644.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1684.00		NIST Webbook
tb	571.55	K	Joback Method
tc	806.48	K	Joback Method
tf	386.33	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.53	J/mol×K	571.55	Joback Method
cpg	523.86	J/mol×K	610.71	Joback Method
cpg	544.56	J/mol×K	649.86	Joback Method
cpg	564.09	J/mol×K	689.02	Joback Method
cpg	582.88	J/mol×K	728.17	Joback Method
cpg	601.40	J/mol×K	767.33	Joback Method
cpg	620.08	J/mol×K	806.48	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=C470406&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume