Thujone

Other names:	Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-, [1S-(1«alpha»,4«alpha»,5«alpha»)]-
	«alpha»-Thujone
	Thujone, cis
	3-Thujanone, (1S,4R,5R)-(-)-
	Thujon
	3-Thujanone, (-)-
	l-Thujone
	4-Methyl-1-(1-methylethyl)bicyclo[3.1.0]hexan-3-one-, (1S,4R,5R)-
	3-Thujone
	cis-Thujone
	(Z)-Thujone
	(-)-Thujone
	Bicyclo(3.1.0)hexan-3-one, 4-methyl-1-(1-methylethyl)-, (1S,4R,5R)-
	NSC 93742
	1-isopropyl-4-methylbicyclo[3.1.0]hexan-3-one
Inchi:	InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-8H,4-5H2,1-3H3/t7-,8-,10+/m1/s1
InchiKey:	USMNOWBWPHYOEA-MRTMQBJTSA-N
Formula:	C10H16O
SMILES:	CC1C(=O)CC2(C(C)C)CC12
Mol. weight [g/mol]:	152.23
CAS:	546-80-5

Physical Properties

Property code	Value	Unit	Source
gf	16.59	kJ/mol	Joback Method
hf	-252.21	kJ/mol	Joback Method
hfus	8.69	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1084.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1102.00		NIST Webbook

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rinpol	1102.00	NIST Webbook
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rinpol	1111.00	NIST Webbook
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ripol	1399.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1421.00		NIST Webbook
tb	504.63	K	Joback Method
tc	724.49	K	Joback Method
tf	311.22	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.27	J/mol×K	504.63	Joback Method
cpg	342.10	J/mol×K	541.27	Joback Method
cpg	358.73	J/mol×K	577.92	Joback Method
cpg	374.30	J/mol×K	614.56	Joback Method

cpg	388.94	J/mol×K	651.20	Joback Method
cpg	402.80	J/mol×K	687.84	Joback Method
cpg	416.01	J/mol×K	724.49	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=C546805&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