Bicyclo[3.1.0]hexan-3-one, 4-methyl-1-(1-methylethyl)-, [1S-(1«alpha»,4«beta»,5«alpha»)]-

Other names:	«beta»-Thujone
	Isothujone
	3-Thujanone, (1S,4S,5R)-(+)-
	(+)-Isothujone
	D-«beta»-Thujone
	D-Isothujone
	Thujone, (+)-
	(+)-Thujone
	(+)-«beta»-Thujone
	1-Isopropyl-4-methylbicyclo[3.1.0]hexan-3-one-, (1S,4S,5R)-
	(E)-Thujone
	Thujone trans
	trans-Thujone
	cis-Thujone (CAS)
	NSC 67392
	trans-thujone («beta»-thujone)
	(d) 1-isopropyl-4-methylbicyclo[3.1.0]hexan-3-one (thujone)
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-HUWCLSLFSA-N
Formula:	C10H16O
SMILES:	CC1C(=O)CC2(C(C)C)CC12
Mol. weight [g/mol]:	152.23
CAS:	471-15-8

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	1114.00		NIST Webbook
rinpol	1121.30		NIST Webbook
rinpol	1095.00		NIST Webbook

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ripol	1426.00		NIST Webbook
ripol	1422.00		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	402.80	J/mol×K	687.84	Joback Method
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	416.01	J/mol×K	724.49	Joback Method
hvapt	51.80	kJ/mol	392.50	NIST Webbook

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=C471158&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

hvapt:	Enthalpy of vaporization at a given temperature
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