Bicyclo[3.1.0]hexan-3-ol, 4-methyl-1-(1-methylethyl)-

Other names: Isothujol
«alpha»-Thujol
3-Thujol

Inchi: InChI=1S/C10H18O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-9,11H,4-5H2,1-3H3

InchiKey: DZVXRFMREAADPP-UHFFFAOYSA-N

Formula: C10H18O

SMILES: CC1C(O)CC2(C(C)C)CC12

Mol. weight [g/mol]: 154.25

CAS: 513-23-5

Physical Properties

Property code	Value	Unit	Source
gf	-5.35	kJ/mol	Joback Method
hf	-287.08	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	52.20	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.049		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1575.00		NIST Webbook
tb	524.32	K	Joback Method
tc	714.97	K	Joback Method
tf	299.58	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.41	J/mol×K	524.32	Joback Method

cpg	370.07	J/mol×K	556.10	Joback Method
cpg	384.74	J/mol×K	587.87	Joback Method
cpg	398.54	J/mol×K	619.65	Joback Method
cpg	411.57	J/mol×K	651.42	Joback Method
cpg	423.94	J/mol×K	683.20	Joback Method
cpg	435.75	J/mol×K	714.97	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=C513235&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