Thujol

Other names: Thujyl alcohol
Thujanol
(1«alpha»,3«alpha»,4«alpha»,5«alpha»)-4-methyl-1-(1-methylethyl)bicyclo[3.1.0]hexan-3
Inchi: InChI=1S/C10H18O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-9,11H,4-5H2,1-3H3/t7?,8?,9-,10
InchiKey: DZVXRFMREAADPP-OWTMBLHMSA-N
Formula: C10H18O
SMILES: CC1C(O)CC2(C(C)C)CC12
Mol. weight [g/mol]: 154.25
CAS: 35732-37-7

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	1145.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1100.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1664.00		NIST Webbook

ripol	1638.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1623.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35732377&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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