

Thujopsan-2-«alpha»-ol

Other names:	Thujopsan-2a-ol
Inchi:	InChI=1S/C15H26O/c1-12(2)6-5-7-13(3)8-9-14(4,16)11-10-15(11,12)13/h11,16H,5-10H2
InchiKey:	YTLMZAPWDFQBAI-LSPKCOCLSA-N
Formula:	C15H26O
SMILES:	CC1(O)CCC2(C)CCCC(C)(C)C23CC13
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	59.27	kJ/mol	Joback Method
hf	-278.80	kJ/mol	Joback Method
hfus	5.85	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.754		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1594.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1594.00		NIST Webbook
tb	655.16	K	Joback Method
tc	876.31	K	Joback Method
tf	453.53	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.59	J/molxK	655.16	Joback Method
cpg	610.07	J/molxK	692.02	Joback Method
cpg	629.03	J/molxK	728.88	Joback Method
cpg	647.94	J/molxK	765.73	Joback Method

cpg	667.27	J/mol×K	802.59	Joback Method
cpg	687.47	J/mol×K	839.45	Joback Method
cpg	709.02	J/mol×K	876.31	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=R201506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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