

3-Thujanol

Other names:	Thujan-3-ol 3-Thujanol (neoisothujanol)
Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)10(9,11)6-9/h7-8,11H,4-6H2,1-3H3
InchiKey:	IKXCCPWTSIENLL-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC1CCC2(C(C)C)CC12O
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
gf	-3.13	kJ/mol	Joback Method
hf	-251.50	kJ/mol	Joback Method
hfus	6.97	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.194		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1166.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1595.00		NIST Webbook
tb	529.23	K	Joback Method
tc	727.62	K	Joback Method
tf	327.72	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.14	J/mol×K	529.23	Joback Method
cpg	368.19	J/mol×K	562.29	Joback Method
cpg	382.12	J/mol×K	595.36	Joback Method
cpg	395.11	J/mol×K	628.42	Joback Method
cpg	407.37	J/mol×K	661.49	Joback Method
cpg	419.07	J/mol×K	694.55	Joback Method
cpg	430.42	J/mol×K	727.62	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=R199770&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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