Thujan-3-ol

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
hfus	6.97	kJ/mol	Joback Method
logp	2.194		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
rinpol	1161.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1166.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1595.00		NIST Webbook

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199770&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices