

trans-4-Thujanol

Inchi: InChI=1S/C10H18O/c1-7(2)10-5-4-9(3,11)8(10)6-10/h7-8,11H,4-6H2,1-3H3/t8-,9-,10-/m1
InchiKey: KXSDPILWGMGFJMM-OPRDCNLKSA-N
Formula: C10H18O
SMILES: CC(C)C12CCC(C)(O)C1C2
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	1070.00		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1058.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1483.00		NIST Webbook
tb	529.23	K	Joback Method
tc	727.62	K	Joback Method
tf	327.72	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.14	J/molxK	529.23	Joback Method
cpg	368.19	J/molxK	562.29	Joback Method
cpg	382.12	J/molxK	595.36	Joback Method
cpg	395.11	J/molxK	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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