

iso-3-Thujanol

Other names:	iso-Thujan-3-ol iso-Thujanol
Inchi:	InChI=1S/C10H18O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-9,11H,4-5H2,1-3H3
InchiKey:	DZVXRFMREAADPP-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CC1C(O)CC2(C(C)C)CC12
Mol. weight [g/mol]:	154.25
CAS:	7712-79-0

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	1142.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1138.30		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1135.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1635.00		NIST Webbook
tb	524.32	K	Joback Method
tc	714.97	K	Joback Method
tf	299.58	K	Joback Method
vc	0.518	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7712790&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinol:	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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