cis-Thujopsadiene

Inchi: InChI=1S/C15H22/c1-11-6-9-14(4)8-5-7-13(2,3)15(14)10-12(11)15/h5-7,12H,8-10H2,1-4
InchiKey: HIRCZOSUMSSTDU-UHFFFAOYSA-N
Formula: C15H22
SMILES: CC1=CCC2(C)CC=CC(C)(C)C23CC13
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	259.58	kJ/mol	Joback Method
hf	-17.38	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1468.00		NIST Webbook
tb	570.71	K	Joback Method
tc	808.01	K	Joback Method
tf	387.09	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.77	J/mol×K	570.71	Joback Method
cpg	502.91	J/mol×K	610.26	Joback Method
cpg	522.45	J/mol×K	649.81	Joback Method
cpg	540.85	J/mol×K	689.36	Joback Method
cpg	558.58	J/mol×K	728.91	Joback Method
cpg	576.10	J/mol×K	768.46	Joback Method
cpg	593.88	J/mol×K	808.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R620536&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
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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