

Dihydrosabinene

Other names:	Thujane
Inchi:	InChI=1S/C10H18/c1-7(2)10-5-4-8(3)9(10)6-10/h7-9H,4-6H2,1-3H3
InchiKey:	GCTNBVHDRFKLLK-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC1CCC2(C(C)C)CC12
Mol. weight [g/mol]:	138.25
CAS:	471-12-5

Physical Properties

Property code	Value	Unit	Source
chl	-6312.00	kJ/mol	NIST Webbook
gf	139.18	kJ/mol	Joback Method
hf	-114.51	kJ/mol	Joback Method
hfus	9.18	kJ/mol	Joback Method
hvap	35.83	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	932.00		NIST Webbook
tb	436.81	K	Joback Method
tc	639.14	K	Joback Method
tf	243.00	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.61	J/molxK	436.81	Joback Method
cpg	307.00	J/molxK	470.53	Joback Method
cpg	324.96	J/molxK	504.25	Joback Method
cpg	341.63	J/molxK	537.97	Joback Method
cpg	357.14	J/molxK	571.70	Joback Method
cpg	371.61	J/molxK	605.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C471125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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