

cis-sabinene

Inchi:	InChI=1S/C10H16/c1-7(2)10-5-4-8(3)9(10)6-10/h7,9H,3-6H2,1-2H3/t9-,10-/m0/s1
InchiKey:	NDVASEGYNIMXJL-RGURZIINSA-N
Formula:	C10H16
SMILES:	C=C1CCC2(C(C)C)CC12
Mol. weight [g/mol]:	136.23

Physical Properties

Property code	Value	Unit	Source
gf	199.97	kJ/mol	Joback Method
hf	-9.93	kJ/mol	Joback Method
hfus	6.95	kJ/mol	Joback Method
hvap	36.30	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	1073.00		NIST Webbook
tb	440.64	K	Joback Method
tc	645.23	K	Joback Method
tf	260.92	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.23	J/mol×K	440.64	Joback Method
cpg	290.70	J/mol×K	474.74	Joback Method
cpg	306.80	J/mol×K	508.84	Joback Method
cpg	321.68	J/mol×K	542.93	Joback Method
cpg	335.47	J/mol×K	577.03	Joback Method
cpg	348.30	J/mol×K	611.13	Joback Method
cpg	360.33	J/mol×K	645.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235519&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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