

«gamma»-Cedrene

Inchi:	InChI=1S/C17H30/c1-8-12(2)14-11-16(6)13(3)9-10-17(16,7)15(14,4)5/h8,13-14H,9-11H2
InchiKey:	MAGKTAGHFGHGSY-QBWHZSSQSA-N
Formula:	C17H30
SMILES:	CC=C(C)C1CC2(C)C(C)CCC2(C)C1(C)C
Mol. weight [g/mol]:	234.42

Physical Properties

Property code	Value	Unit	Source
gf	221.63	kJ/mol	Joback Method
hf	-168.80	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method
hvap	49.26	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	5.441		Crippen Method
mcvol	224.370	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
ripol	1649.00		NIST Webbook
ripol	1649.00		NIST Webbook
tb	601.13	K	Joback Method
tc	821.86	K	Joback Method
tf	350.13	K	Joback Method
vc	0.858	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.88	J/mol×K	601.13	Joback Method
cpg	647.12	J/mol×K	637.92	Joback Method
cpg	670.03	J/mol×K	674.71	Joback Method
cpg	691.97	J/mol×K	711.50	Joback Method
cpg	713.28	J/mol×K	748.28	Joback Method
cpg	734.33	J/mol×K	785.07	Joback Method
cpg	755.46	J/mol×K	821.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335887&Units=SI

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
hvp:	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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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