

Geranyl-«alpha»-terpinene

Inchi:	InChI=1S/C20H32/c1-15(2)8-7-9-17(5)10-12-20-14-19(16(3)4)13-11-18(20)6/h8,10,14,16
InchiKey:	ZKIGZHMBLJAPAC-LICLKQGHSA-N
Formula:	C20H32
SMILES:	CC(C)=CCCC(C)=CCC1=C(C)CCC(C(C)C)=C1
Mol. weight [g/mol]:	272.47

Physical Properties

Property code	Value	Unit	Source
gf	321.61	kJ/mol	Joback Method
hf	-90.74	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.762		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
ripol	2223.00		NIST Webbook
ripol	2142.00		NIST Webbook
ripol	2142.00		NIST Webbook
tb	702.12	K	Joback Method
tc	905.98	K	Joback Method
tf	312.78	K	Joback Method
vc	1.018	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.31	J/mol×K	702.12	Joback Method
cpg	768.18	J/mol×K	736.10	Joback Method
cpg	787.90	J/mol×K	770.07	Joback Method

cpg	806.55	J/mol×K	804.05	Joback Method
cpg	824.20	J/mol×K	838.03	Joback Method
cpg	840.91	J/mol×K	872.00	Joback Method
cpg	856.75	J/mol×K	905.98	Joback Method

Sources

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=R517836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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