

2,2,6,7-tetramethylbicyclo-[4.3.0]nona-4,9(1)-dien-

Inchi:	InChI=1S/C13H20O/c1-9-11(14)7-10-8-12(2,3)5-6-13(9,10)4/h5-7,9,11,14H,8H2,1-4H3
InchiKey:	WRBJGCSDYSDMRE-UHFFFAOYSA-N
Formula:	C13H20O
SMILES:	CC1C(O)C=C2CC(C)(C)C=CC21C
Mol. weight [g/mol]:	192.30

Physical Properties

Property code	Value	Unit	Source
gf	30.85	kJ/mol	Joback Method
hf	-242.87	kJ/mol	Joback Method
hfus	15.08	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.916		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
ripol	2033.00		NIST Webbook
tb	609.75	K	Joback Method
tc	819.84	K	Joback Method
tf	375.77	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.15	J/molxK	609.75	Joback Method
cpg	480.88	J/molxK	644.76	Joback Method
cpg	496.73	J/molxK	679.78	Joback Method
cpg	511.91	J/molxK	714.79	Joback Method
cpg	526.61	J/molxK	749.81	Joback Method
cpg	541.04	J/molxK	784.82	Joback Method
cpg	555.40	J/molxK	819.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R297200&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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