

# Pulegone

<b>Other names:</b>	(+)-(R)-Pulegone (+)-4(8)-Para-menthen-3-one (+)-Pulegone (1R)-(+)-p-Menth-4(8)-en-3-one (R)-(+)-Pulegone (R)-Pulegone 1-Isopropylidene-4-methyl-2-cyclohexanone 1-Methyl-4-isopropylidene-3-cyclohexanone 3-Methyl-6-isopropylidenecyclohexanone 4(8)-p-Menthen-3-one, (R)-(+)- 5-Methyl-2-(1-methylethylidene)cyclohexanone, (R)- Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (5R)- Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)- NSC 15334 Pulegon Pulegone, (d) d-Pulegone d-p-Menth-4(8)-en-3-one p-Menth-4(8)-en-3-one p-Menth-4(8)-en-3-one, (R)-(+)-
<b>Inchi:</b>	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h8H,4-6H2,1-3H3/t8-/m0/s1
<b>InchiKey:</b>	NZGWDASTMWDZIW-QMMMGPBSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	CC(C)=C1CCC(C)CC1=O
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	89-82-7

## Physical Properties

Property code	Value	Unit	Source
chl	-5933.30	kJ/mol	NIST Webbook
gf	-27.91	kJ/mol	Joback Method
hf	-266.87	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	62.00	kJ/mol	NIST Webbook
hvap	58.00	kJ/mol	NIST Webbook
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method

mcvol	138.170	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1225.70		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1212.29		NIST Webbook
rinpol	1216.66		NIST Webbook
rinpol	1221.11		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1230.35		NIST Webbook
rinpol	1235.16		NIST Webbook
rinpol	1239.97		NIST Webbook
rinpol	1244.84		NIST Webbook
rinpol	1250.14		NIST Webbook
rinpol	1203.81		NIST Webbook
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rinpol	1235.00		NIST Webbook
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rinpol	1208.00		NIST Webbook
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ripol	1662.00			NIST Webbook
ripol	1662.00			NIST Webbook
tb	497.00 ± 0.50		K	NIST Webbook
tb	497.00 ± 3.00		K	NIST Webbook
tb	497.20		K	NIST Webbook
tc	747.18		K	Joback Method
tf	274.46		K	Joback Method
vc	0.519		m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.93	J/mol×K	672.15	Joback Method
cpg	402.44	J/mol×K	709.67	Joback Method
cpg	321.00	J/mol×K	522.09	Joback Method
cpg	339.06	J/mol×K	559.61	Joback Method
cpg	356.24	J/mol×K	597.12	Joback Method
cpg	372.52	J/mol×K	634.64	Joback Method
cpg	416.08	J/mol×K	747.18	Joback Method
cpl	274.90	J/mol×K	293.30	NIST Webbook
cpl	274.90	J/mol×K	293.30	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	9.09929e+00
Coeff. B	-1.16405e+03
Coeff. C	-2.37423e+02
Temperature range (K), min.	369.53
Temperature range (K), max.	544.74

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C89827&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89827&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure

<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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