Pulegone

Other names:	(+)-(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)-(+)-
Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h8H,4-6H2,1-3H3/t8-/m0/s1
InchiKey:	NZGWDASTMWDZIW-QMMMGPOBSA-N
Formula:	C10H16O
SMILES:	CC(C)=C1CCC(C)CC1=O
Mol. weight [g/mol]:	152.23
CAS:	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	58.00	kJ/mol	NIST Webbook
hvap	62.00	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	1210.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
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ripol	1665.00		NIST Webbook
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ripol	1644.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	497.20	K	NIST Webbook
tb	497.00 ± 0.50	K	NIST Webbook
tb	497.00 ± 3.00	K	NIST Webbook
tc	747.18	K	Joback Method
tf	274.46	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	387.93	J/mol×K	672.15	Joback Method
cpg	402.44	J/mol×K	709.67	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(Pvp) = 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

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=C89827&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
pvap:	Vapor 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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