

Pulegol

Other names:	Cyclohexanol,5-methyl-2-(1-methylethylidene)
Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h8-11H,1,4-6H2,2-3H3
InchiKey:	ZYTMANIQRDEHIO-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=C(C)C1CCC(C)CC1O
Mol. weight [g/mol]:	154.25
CAS:	529-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-15.18	kJ/mol	Joback Method
hf	-272.68	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.360		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	527.15	K	Joback Method
tc	719.80	K	Joback Method
tf	246.46	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	350.71	J/mol×K	527.15	Joback Method
cpg	367.51	J/mol×K	559.26	Joback Method
cpg	383.50	J/mol×K	591.37	Joback Method
cpg	398.69	J/mol×K	623.47	Joback Method
cpg	413.11	J/mol×K	655.58	Joback Method
cpg	426.76	J/mol×K	687.69	Joback Method
cpg	439.67	J/mol×K	719.80	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=C529022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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