dl-Isopulegol

Other names: Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, (1«alpha»,2«beta»,5«alpha»)-(.+/-.)-
Isopulegol, (.+/-.)-
2-Isopropenyl-5-methylcyclohexanol, (1«alpha»,2«beta»,5«alpha»)-
Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, (1R,2S,5R)-rel-
(±)-(1«alpha»,2«beta»,5«alpha»)-5-methyl-2-(1-methylvinyl)cyclohexan-1-ol
iso-Isopulegol

Inchi: InChI=1S/C10H18O/c1-7(2)9-5-4-8(3)6-10(9)11/h8-11H,1,4-6H2,2-3H3/t8-,9-,10+/m0/s1

InchiKey: ZYTMANIQRDEHIO-LPEHRKFASA-N

Formula: C10H18O

SMILES: C=C(C)C1CCC(C)CC1O

Mol. weight [g/mol]: 154.25

CAS: 59905-53-2

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	1157.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1159.00		NIST Webbook

rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1146.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	527.15	K	Joback Method
tc	719.80	K	Joback Method
tf	246.46	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C59905532&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
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