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 dl-isopulgeol

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: 50373-36-9

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	1159.00		NIST Webbook
rinpol	1167.00		NIST Webbook
ripol	1606.00		NIST Webbook
tb	485.15 ± 1.00	K	NIST Webbook
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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50373369&Units=SI
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

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