

cis-Isopulegone

Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h8-9H,1,4-6H2,2-3H3/t8-,9-/m1/s1
InchiKey:	RMIANEGNSBUGDJ-RKDXNWHRSA-N
Formula:	C10H16O
SMILES:	C=C(C)C1CCC(C)CC1=O
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	6.76	kJ/mol	Joback Method
hf	-237.81	kJ/mol	Joback Method
hfus	11.48	kJ/mol	Joback Method
hvap	41.63	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1159.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1583.00		NIST Webbook
ripol	1583.00		NIST Webbook
tb	507.46	K	Joback Method
tc	729.79	K	Joback Method
tf	258.10	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.01	J/mol×K	507.46	Joback Method
cpg	339.03	J/mol×K	544.51	Joback Method

cpg	357.13	J/mol×K	581.57	Joback Method
cpg	374.31	J/mol×K	618.62	Joback Method
cpg	390.57	J/mol×K	655.68	Joback Method
cpg	405.90	J/mol×K	692.73	Joback Method
cpg	420.31	J/mol×K	729.79	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=R323314&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

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