

cis-Isodihydrocarvone

Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(11)6-9/h8-9H,1,4-6H2,2-3H3/t8-,9+/m1/s1
InchiKey:	AZOCECCLWFDTAP-BDAKNGLRSA-N
Formula:	C10H16O
SMILES:	C=C(C)C1CCC(C)C(=O)C1
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
ripol	1196.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236785&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

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