

cis-(2,3,3a,7a-Tetrahydro-1H-indene-4-carbaldehy

Inchi:	InChI=1S/C10H12O/c11-7-9-5-1-3-8-4-2-6-10(8)9/h1,3,5,7-8,10H,2,4,6H2/t8-,10+/m1/s1
InchiKey:	NRPGDWVRKOJMEE-SCZZXKLOSA-N
Formula:	C10H12O
SMILES:	O=CC1=CC=CC2CCCC12
Mol. weight [g/mol]:	148.20

Physical Properties

Property code	Value	Unit	Source
gf	69.29	kJ/mol	Joback Method
hf	-104.10	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	46.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.098		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
ripol	1270.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1876.00		NIST Webbook
tb	506.45	K	Joback Method
tc	730.39	K	Joback Method
tf	283.82	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.32	J/molxK	506.45	Joback Method
cpg	352.11	J/molxK	693.07	Joback Method
cpg	339.93	J/molxK	655.74	Joback Method
cpg	326.82	J/molxK	618.42	Joback Method
cpg	312.72	J/molxK	581.10	Joback Method
cpg	297.58	J/molxK	543.77	Joback Method
cpg	363.43	J/molxK	730.39	Joback Method

dvisc	0.0006098	Paxs	506.45	Joback Method
dvisc	0.0006920	Paxs	469.34	Joback Method
dvisc	0.0008026	Paxs	432.24	Joback Method
dvisc	0.0009570	Paxs	395.13	Joback Method
dvisc	0.0011837	Paxs	358.03	Joback Method
dvisc	0.0015377	Paxs	320.93	Joback Method
dvisc	0.0021391	Paxs	283.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586708&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
dvisc:	Dynamic viscosity
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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