

1,3-Cyclohexadiene-1-carboxaldehyde

Inchi:	InChI=1S/C7H8O/c8-6-7-4-2-1-3-5-7/h1-2,4,6H,3,5H2
InchiKey:	LQXUYPKOOOUVJB-UHFFFAOYSA-N
Formula:	C7H8O
SMILES:	O=CC1=CC=CCC1
Mol. weight [g/mol]:	108.14

Physical Properties

Property code	Value	Unit	Source
gf	-9.01	kJ/mol	Joback Method
hf	-94.64	kJ/mol	Joback Method
hfus	8.99	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.462		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
ripol	1184.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1603.00		NIST Webbook
tb	435.74	K	Joback Method
tc	652.26	K	Joback Method
tf	236.31	K	Joback Method
vc	0.350	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.33	J/molxK	435.74	Joback Method
cpg	180.86	J/molxK	471.83	Joback Method
cpg	191.69	J/molxK	507.91	Joback Method
cpg	201.86	J/molxK	544.00	Joback Method
cpg	211.39	J/molxK	580.09	Joback Method
cpg	220.31	J/molxK	616.18	Joback Method

cpg	228.65	J/mol×K	652.26	Joback Method
dvisc	0.0038609	Paxs	236.31	Joback Method
dvisc	0.0019681	Paxs	269.55	Joback Method
dvisc	0.0011632	Paxs	302.79	Joback Method
dvisc	0.0007628	Paxs	336.02	Joback Method
dvisc	0.0005397	Paxs	369.26	Joback Method
dvisc	0.0004044	Paxs	402.50	Joback Method
dvisc	0.0003166	Paxs	435.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R432745&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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