

1-Cyclopentene-1-carboxaldehyde

Inchi:	InChI=1S/C6H8O/c7-5-6-3-1-2-4-6/h3,5H,1-2,4H2
InchiKey:	RALDHUZXJKFQB-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	O=CC1=CCCC1
Mol. weight [g/mol]:	96.13
CAS:	6140-65-4

Physical Properties

Property code	Value	Unit	Source
gf	-35.29	kJ/mol	Joback Method
hf	-125.62	kJ/mol	Joback Method
hfus	7.28	kJ/mol	Joback Method
hvap	37.19	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.296		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
tb	419.20	K	NIST Webbook
tc	617.48	K	Joback Method
tf	227.80	K	Joback Method
vc	0.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.85	J/mol×K	409.43	Joback Method
cpg	157.54	J/mol×K	444.11	Joback Method
cpg	167.60	J/mol×K	478.78	Joback Method
cpg	177.07	J/mol×K	513.46	Joback Method
cpg	185.97	J/mol×K	548.13	Joback Method
cpg	194.33	J/mol×K	582.81	Joback Method
cpg	202.17	J/mol×K	617.48	Joback Method

dvisc	0.0030456	Paxs	227.80	Joback Method
dvisc	0.0017468	Paxs	258.07	Joback Method
dvisc	0.0011259	Paxs	288.34	Joback Method
dvisc	0.0007889	Paxs	318.62	Joback Method
dvisc	0.0005879	Paxs	348.89	Joback Method
dvisc	0.0004592	Paxs	379.16	Joback Method
dvisc	0.0003721	Paxs	409.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.20	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6140654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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