

Cyclopentanecarboxaldehyde

Other names:	Cyclopentanealdehyde Cyclopentylformaldehyde Formylcyclopentane Cyclopentyl aldehyde Cyclopentane-1-carboxaldehyde cyclopentanecarbaldehyde
Inchi:	InChI=1S/C6H10O/c7-5-6-3-1-2-4-6/h5-6H,1-4H2
InchiKey:	VELDYOPRLMJFIK-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	O=CC1CCCC1
Mol. weight [g/mol]:	98.14
CAS:	872-53-7

Physical Properties

Property code	Value	Unit	Source
gf	-63.33	kJ/mol	Joback Method
hf	-192.27	kJ/mol	Joback Method
hfus	7.52	kJ/mol	Joback Method
hvap	35.93	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.375		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
rinpol	857.00		NIST Webbook
ripol	1170.00		NIST Webbook
ripol	1171.00		NIST Webbook
tb	400.62	K	Joback Method
tc	604.41	K	Joback Method
tf	210.28	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	159.16	J/molxK	400.62	Joback Method
cpg	171.99	J/molxK	434.58	Joback Method
cpg	184.14	J/molxK	468.55	Joback Method
cpg	195.63	J/molxK	502.51	Joback Method
cpg	206.48	J/molxK	536.48	Joback Method
cpg	216.72	J/molxK	570.44	Joback Method
cpg	226.37	J/molxK	604.41	Joback Method
dvisc	0.0036458	Paxs	210.28	Joback Method
dvisc	0.0019804	Paxs	242.00	Joback Method
dvisc	0.0012392	Paxs	273.73	Joback Method
dvisc	0.0008548	Paxs	305.45	Joback Method
dvisc	0.0006323	Paxs	337.17	Joback Method
dvisc	0.0004926	Paxs	368.90	Joback Method
dvisc	0.0003992	Paxs	400.62	Joback Method

Sources

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=C872537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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