

Cyclopentaneacetic acid

Other names:	Cyclopentylacetic acid
Inchi:	InChI=1S/C7H12O2/c8-7(9)5-6-3-1-2-4-6/h6H,1-5H2,(H,8,9)
InchiKey:	YVHAIVPPUIZFBA-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	O=C(O)CC1CCCC1
Mol. weight [g/mol]:	128.17
CAS:	1123-00-8

Physical Properties

Property code	Value	Unit	Source
gf	-221.13	kJ/mol	Joback Method
hf	-392.14	kJ/mol	Joback Method
hfus	13.51	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.651		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	501.20	K	NIST Webbook
tc	716.27	K	Joback Method
tf	290.30	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.06	J/mol×K	520.89	Joback Method
cpg	304.11	J/mol×K	683.71	Joback Method
cpg	294.52	J/mol×K	651.14	Joback Method
cpg	284.34	J/mol×K	618.58	Joback Method
cpg	273.56	J/mol×K	586.02	Joback Method
cpg	262.14	J/mol×K	553.45	Joback Method
cpg	313.13	J/mol×K	716.27	Joback Method
dvisc	0.0002179	Pa×s	520.89	Joback Method

dvisc	0.0003367	Pa×s	482.46	Joback Method
dvisc	0.0005611	Pa×s	444.03	Joback Method
dvisc	0.0010300	Pa×s	405.60	Joback Method
dvisc	0.0021470	Pa×s	367.16	Joback Method
dvisc	0.0053141	Pa×s	328.73	Joback Method
dvisc	0.0167199	Pa×s	290.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.70	K	3.10	NIST Webbook

Sources

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=C1123008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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