Cyclopentylcarboxylic acid

Other names: Cyclopentanecarboxylic acid
Cyclopentylmethanoic acid
Inchi: InChI=1S/C6H10O2/c7-6(8)5-3-1-2-4-5/h5H,1-4H2,(H,7,8)
InchiKey: JBDSSBMEKXHSJF-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: O=C(O)C1CCCC1
Mol. weight [g/mol]: 114.14
CAS: 3400-45-1

Physical Properties

Property code	Value	Unit	Source
affp	817.40	kJ/mol	NIST Webbook
basg	786.40	kJ/mol	NIST Webbook
gf	-229.55	kJ/mol	Joback Method
hf	-371.50	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	52.63	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.261		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
tb	489.20	K	NIST Webbook
tc	695.98	K	Joback Method
tf	279.03	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.79	J/mol×K	498.01	Joback Method
cpg	217.91	J/mol×K	531.00	Joback Method
cpg	228.41	J/mol×K	564.00	Joback Method
cpg	238.31	J/mol×K	596.99	Joback Method
cpg	247.65	J/mol×K	629.99	Joback Method

cpg	256.44	J/mol×K	662.98	Joback Method
cpg	264.70	J/mol×K	695.98	Joback Method
dvisc	0.0192641	Pa×s	279.03	Joback Method
dvisc	0.0061558	Pa×s	315.53	Joback Method
dvisc	0.0024921	Pa×s	352.02	Joback Method
dvisc	0.0011957	Pa×s	388.52	Joback Method
dvisc	0.0006508	Pa×s	425.02	Joback Method
dvisc	0.0003900	Pa×s	461.51	Joback Method
dvisc	0.0002519	Pa×s	498.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	1.50	NIST Webbook
tbrp	389.50 ± 0.50	K	2.80	NIST Webbook

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=C3400451&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
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