Cyclobutylcarboxylic acid

Other names: Cyclobutanecarboxylic acid
Inchi: InChI=1S/C5H8O2/c6-5(7)4-2-1-3-4/h4H,1-3H2,(H,6,7)
InchiKey: TXWOGHSRPAYOML-UHFFFAOYSA-N
Formula: C5H8O2
SMILES: O=C(O)C1CCC1
Mol. weight [g/mol]: 100.12
CAS: 3721-95-7

Physical Properties

Property code	Value	Unit	Source
affp	817.40	kJ/mol	NIST Webbook
basg	786.40	kJ/mol	NIST Webbook
chl	-2684.00	kJ/mol	NIST Webbook
chl	-2685.60 ± 1.80	kJ/mol	NIST Webbook
gf	-225.87	kJ/mol	Joback Method
hf	-344.70	kJ/mol	Joback Method
hfl	-425.30 ± 1.80	kJ/mol	NIST Webbook
hfus	10.43	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Joback Method
ie	10.35	eV	NIST Webbook
log10ws	-0.67		Crippen Method
logp	0.871		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	987.00		NIST Webbook
ripol	1885.00		NIST Webbook
ripol	1831.00		NIST Webbook
tb	468.20	K	NIST Webbook
tc	664.03	K	Joback Method
tf	266.05 ± 1.00	K	NIST Webbook
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.65	J/mol×K	470.86	Joback Method
cpg	207.96	J/mol×K	631.84	Joback Method
cpg	200.66	J/mol×K	599.64	Joback Method
cpg	192.90	J/mol×K	567.45	Joback Method
cpg	184.66	J/mol×K	535.25	Joback Method
cpg	175.92	J/mol×K	503.06	Joback Method
cpg	214.83	J/mol×K	664.03	Joback Method
dvisc	0.0003513	Pa×s	470.86	Joback Method
dvisc	0.0005212	Pa×s	437.60	Joback Method
dvisc	0.0008253	Pa×s	404.33	Joback Method
dvisc	0.0014190	Pa×s	371.07	Joback Method
dvisc	0.0027146	Pa×s	337.81	Joback Method
dvisc	0.0059837	Pa×s	304.54	Joback Method
dvisc	0.0160108	Pa×s	271.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.00 ± 2.00	K	2.00	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=C3721957&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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