3-Methylenecyclobutanecarboxylic acid

Inchi: InChI=1S/C6H8O2/c1-4-2-5(3-4)6(7)8/h5H,1-3H2,(H,7,8)
InchiKey: NNKLICLIBKMDOY-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: C=C1CC(C(=O)O)C1
Mol. weight [g/mol]: 112.13
CAS: 15760-36-8

Physical Properties

Property code	Value	Unit	Source
gf	-164.37	kJ/mol	Joback Method
hf	-281.10	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	52.62	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	1.037		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
tb	492.90	K	Joback Method
tc	685.45	K	Joback Method
tf	296.23	K	Joback Method
vc	0.330	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.51	J/mol×K	492.90	Joback Method
cpg	230.70	J/mol×K	653.36	Joback Method
cpg	223.56	J/mol×K	621.27	Joback Method
cpg	215.99	J/mol×K	589.18	Joback Method
cpg	207.97	J/mol×K	557.08	Joback Method
cpg	199.49	J/mol×K	524.99	Joback Method
cpg	237.44	J/mol×K	685.45	Joback Method
dvisc	0.0003288	Pa×s	492.90	Joback Method
dvisc	0.0004642	Pa×s	460.12	Joback Method

dvisc	0.0006910	Pa×s	427.34	Joback Method
dvisc	0.0010989	Pa×s	394.56	Joback Method
dvisc	0.0019007	Pa×s	361.79	Joback Method
dvisc	0.0036670	Pa×s	329.01	Joback Method
dvisc	0.0081819	Pa×s	296.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15760368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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