

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/molxK	492.90	Joback Method
cpg	199.49	J/molxK	524.99	Joback Method
cpg	207.97	J/molxK	557.08	Joback Method
cpg	215.99	J/molxK	589.18	Joback Method
cpg	223.56	J/molxK	621.27	Joback Method
cpg	230.70	J/molxK	653.36	Joback Method
cpg	237.44	J/molxK	685.45	Joback Method
dvisc	0.0081819	Paxs	296.23	Joback Method
dvisc	0.0036670	Paxs	329.01	Joback Method

dvisc	0.0019007	Paxs	361.79	Joback Method
dvisc	0.0010989	Paxs	394.56	Joback Method
dvisc	0.0006910	Paxs	427.34	Joback Method
dvisc	0.0004642	Paxs	460.12	Joback Method
dvisc	0.0003288	Paxs	492.90	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=C15760368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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