3-Methylenecyclopropane-trans-1,2-dicarboxylic acid

Other names: trans-1-Methylene cyclopropane-2,3-dicarboxylic acid
1,2-Cyclopropanedicarboxylic acid, 3-methylene-, trans-
3-Methylenecyclopropane-1,2-dicarboxylic acid, trans-
3-Methylene-cyclopropane-1,2-dicarboxylic acid
Feist'S acid
dl-3-Methylenecyclopropane-trans-1,2-dicarboxylic acid
trans-3-methylenecyclopropane-1,2-dicarboxylic acid

Inchi: InChI=1S/C6H6O4/c1-2-3(5(7)8)4(2)6(9)10/h3-4H,1H2,(H,7,8)(H,9,10)/t3-,4-/m1/s1

InchiKey: XZVHROKAQFFOCA-QWWZWVQMSA-N

Formula: C6H6O4

SMILES: C=C1C(C(=O)O)C1C(=O)O

Mol. weight [g/mol]: 142.11

CAS: 499-02-5

Physical Properties

Property code	Value	Unit	Source
gf	-425.72	kJ/mol	Joback Method
hf	-560.09	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	75.56	kJ/mol	Joback Method
log10ws	0.20		Crippen Method
logp	-0.042		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
tb	630.01	K	Joback Method
tc	814.58	K	Joback Method
tf	406.26	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.93	J/mol×K	630.01	Joback Method
cpg	270.47	J/mol×K	783.82	Joback Method

cpg	265.42	J/mol×K	753.06	Joback Method
cpg	260.06	J/mol×K	722.29	Joback Method
cpg	254.37	J/mol×K	691.53	Joback Method
cpg	248.33	J/mol×K	660.77	Joback Method
cpg	275.23	J/mol×K	814.58	Joback Method
dvisc	0.0001224	Pa×s	630.01	Joback Method
dvisc	0.0001805	Pa×s	592.72	Joback Method
dvisc	0.0002805	Pa×s	555.43	Joback Method
dvisc	0.0004644	Pa×s	518.13	Joback Method
dvisc	0.0008314	Pa×s	480.84	Joback Method
dvisc	0.0016417	Pa×s	443.55	Joback Method
dvisc	0.0036729	Pa×s	406.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C499025&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