

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)
InchiKey:	XZVHROKAQFFOCA-UHFFFAOYSA-N
Formula:	C6H6O4
SMILES:	C=C1C(C(=O)O)C1C(=O)O
Mol. weight [g/mol]:	142.11
CAS:	45786-15-0

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.93	J/molxK	630.01	Joback Method
cpg	270.47	J/molxK	783.82	Joback Method
cpg	265.42	J/molxK	753.06	Joback Method
cpg	260.06	J/molxK	722.29	Joback Method
cpg	254.37	J/molxK	691.53	Joback Method
cpg	248.33	J/molxK	660.77	Joback Method
cpg	275.23	J/molxK	814.58	Joback Method
dvisc	0.0001224	Paxs	630.01	Joback Method
dvisc	0.0001805	Paxs	592.72	Joback Method

dvisc	0.0002805	Paxs	555.43	Joback Method
dvisc	0.0004644	Paxs	518.13	Joback Method
dvisc	0.0008314	Paxs	480.84	Joback Method
dvisc	0.0016417	Paxs	443.55	Joback Method
dvisc	0.0036729	Paxs	406.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C45786150&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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