

1,3-Dioxane-4,6-dione, 2,2-dimethyl-

Other names: Malonic acid, cyclic isopropylidene ester
Cyclic isopropylidene malonate
Isopropylidene malonate
Meldrum's acid
2,2-Dimethyl-1,3-dioxane-4,6-dione
Meldrums acid
2,2-Dimethyl-m-dioxane-4,6-dione
4,6-Diketo-2,2-dimethyl-1,3-dioxane
2,2-Dimethyl-1,3-dioxan-4,6-dione
m-Dioxane-4,6-dione, 2,2-dimethyl-
2,2-Dimethyl-4,6-dioxo-m-dioxane
2,2-Dimethyl-4,6-dioxo-1,3-dioxane
NSC 71902

Inchi: InChI=1S/C6H8O4/c1-6(2)9-4(7)3-5(8)10-6/h3H2,1-2H3

InchiKey: GXHFUVWIGNLZSC-UHFFFAOYSA-N

Formula: C6H8O4

SMILES: CC1(C)OC(=O)CC(=O)O1

Mol. weight [g/mol]: 144.13

CAS: 2033-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-398.82	kJ/mol	Joback Method
hf	-637.01	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	45.74	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.213		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	546.01	K	Joback Method
tc	797.64	K	Joback Method
tf	378.24	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.53	J/mol×K	546.01	Joback Method
cpg	255.58	J/mol×K	587.95	Joback Method
cpg	268.00	J/mol×K	629.89	Joback Method
cpg	279.83	J/mol×K	671.83	Joback Method
cpg	291.14	J/mol×K	713.77	Joback Method
cpg	301.97	J/mol×K	755.70	Joback Method
cpg	312.39	J/mol×K	797.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2033241&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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