

2,5-Furandione, dihydro-3-methylene-

Other names:	Itaconic anhydride Itaconic acid anhydride Methylenesuccinic anhydride Succinic anhydride, methylene- Dihydro-3-methylene-2,5-furandione 2-Methylenesuccinic anhydride
Inchi:	InChI=1S/C5H4O3/c1-3-2-4(6)8-5(3)7/h1-2H2
InchiKey:	OFNISBHGPNTMS-UHFFFAOYSA-N
Formula:	C5H4O3
SMILES:	C=C1CC(=O)OC1=O
Mol. weight [g/mol]:	112.08
CAS:	2170-03-8

Physical Properties

Property code	Value	Unit	Source
gf	-242.74	kJ/mol	Joback Method
hf	-388.87	kJ/mol	Joback Method
hfus	7.41	kJ/mol	Joback Method
hvap	40.45	kJ/mol	Joback Method
ie	10.68	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
log10ws	-0.30		Crippen Method
logp	0.016		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	5065.79	kPa	Joback Method
ripol	967.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	495.50	K	Joback Method
tc	737.16	K	Joback Method
tf	341.15 ± 1.00	K	NIST Webbook
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.64	J/mol×K	495.50	Joback Method
cpg	164.92	J/mol×K	535.78	Joback Method
cpg	173.96	J/mol×K	576.05	Joback Method
cpg	182.70	J/mol×K	616.33	Joback Method
cpg	191.08	J/mol×K	656.60	Joback Method
cpg	199.04	J/mol×K	696.88	Joback Method
cpg	206.54	J/mol×K	737.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	1.60	NIST Webbook
tbrp	412.70	K	4.00	NIST Webbook

Sources

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=C2170038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvp:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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