1-Cyclopenten-3,4-dione

Other names: cyclopent-3-en-1,2-dione
Inchi: InChI=1S/C5H4O2/c6-4-2-1-3-5(4)7/h1-2H,3H2
InchiKey: WMNNFUMNTPIROQ-UHFFFAOYSA-N
Formula: C5H4O2
SMILES: O=C1C=CCC1=O
Mol. weight [g/mol]: 96.08

Physical Properties

Property code	Value	Unit	Source
gf	-179.74	kJ/mol	Joback Method
hf	-283.33	kJ/mol	Joback Method
hfus	1.81	kJ/mol	Joback Method
hvap	36.08	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	0.084		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
ripol	1580.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1578.00		NIST Webbook
tb	468.55	K	Joback Method
tc	712.77	K	Joback Method
tf	298.45	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.50	J/mol×K	468.55	Joback Method
cpg	141.13	J/mol×K	509.25	Joback Method
cpg	150.46	J/mol×K	549.96	Joback Method
cpg	159.44	J/mol×K	590.66	Joback Method
cpg	168.03	J/mol×K	631.36	Joback Method

cpg	176.19	J/mol×K	672.07	Joback Method
cpg	183.87	J/mol×K	712.77	Joback Method

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=R318619&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume