

2,5(1H,3H)-Pentalenedione, tetrahydro-, cis-

Other names:	cis-Bicyclo[3.3.0]octane-3,7-dione cis-Bicyclo(3.3.0)octane-3,7-dione Tetrahydro-2,5(1H,3H)-pentalenedione, cis- cis-tetrahydropentalene-2,5(1H,3H)-dione
Inchi:	InChI=1S/C8H10O2/c9-7-1-5-2-8(10)4-6(5)3-7/h5-6H,1-4H2/t5-,6+
InchiKey:	HAFQHNGZPQYKFF-OLQVQODUSA-N
Formula:	C8H10O2
SMILES:	O=C1CC2CC(=O)CC2C1
Mol. weight [g/mol]:	138.16
CAS:	51716-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-131.40	kJ/mol	Joback Method
hf	-350.57	kJ/mol	Joback Method
hfus	7.57	kJ/mol	Joback Method
hvap	42.07	kJ/mol	Joback Method
ie	9.78	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
log10ws	-1.04		Crippen Method
logp	0.945		Crippen Method
mcvol	105.000	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	540.10	K	Joback Method
tc	787.01	K	Joback Method
tf	345.20	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.56	J/molxK	540.10	Joback Method
cpg	278.14	J/molxK	581.25	Joback Method

cpg	293.78	J/mol×K	622.40	Joback Method
cpg	308.48	J/mol×K	663.55	Joback Method
cpg	322.25	J/mol×K	704.71	Joback Method
cpg	335.07	J/mol×K	745.86	Joback Method
cpg	346.96	J/mol×K	787.01	Joback Method

Sources

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=C51716633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	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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