

cyclopent-3-en-1,2-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
hfus	1.81	kJ/mol	Joback Method
logp	0.084		Crippen Method
mcpvol	69.290	ml/mol	McGowan 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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R318619&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/80-846-4/cyclopent-3-en-1-2-dione.pdf>

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