

cis-3,4-Dihydro-3,4-dimethyl-2,5-furandione

Inchi:	InChI=1S/C6H8O3/c1-3-4(2)6(8)9-5(3)7/h3-4H,1-2H3/t3-,4+
InchiKey:	HXFIRQHMJBTRV-ZXZARUISSA-N
Formula:	C6H8O3
SMILES:	CC1C(=O)OC(=O)C1C
Mol. weight [g/mol]:	128.13
CAS:	16844-07-8

Physical Properties

Property code	Value	Unit	Source
chs	-2846.40 ± 1.40	kJ/mol	NIST Webbook
gf	-302.82	kJ/mol	Joback Method
hf	-534.43	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	41.90	kJ/mol	Joback Method
log10ws	-0.38		Crippen Method
logp	0.342		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	509.88	K	Joback Method
tc	744.55	K	Joback Method
tf	327.05	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.61	J/molxK	509.88	Joback Method
cpg	230.78	J/molxK	548.99	Joback Method
cpg	243.53	J/molxK	588.10	Joback Method
cpg	255.78	J/molxK	627.21	Joback Method
cpg	267.49	J/molxK	666.32	Joback Method
cpg	278.58	J/molxK	705.44	Joback Method
cpg	289.01	J/molxK	744.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16844078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

chs:	Standard solid enthalpy of combustion
cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	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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