trans-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-/m1/s1
InchiKey: HXFIRQHMXJBTRV-QWWZWVQMSA-N
Formula: C6H8O3
SMILES: CC1C(=O)OC(=O)C1C
Mol. weight [g/mol]: 128.13
CAS: 35392-94-0

Physical Properties

Property code	Value	Unit	Source
chs	-2839.00 ± 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/mol×K	509.88	Joback Method
cpg	230.78	J/mol×K	548.99	Joback Method
cpg	243.53	J/mol×K	588.10	Joback Method
cpg	255.78	J/mol×K	627.21	Joback Method
cpg	267.49	J/mol×K	666.32	Joback Method
cpg	278.58	J/mol×K	705.44	Joback Method
cpg	289.01	J/mol×K	744.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C35392940&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume