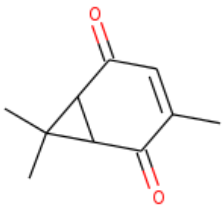
3,7,7-Trimethylbicyclo[4.1.0]hept-3-ene-2,5-dione

InChI:
InChI=1S/C10H12O2/c1-5-4-6(11)7-8(9(5)12)10(7,2)3/h4,7-8H,1-3H3
InChI Key: BBRJZZUFDYMNIY-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC1=CC(=O)C2C(C1=O)C2(C)C
Molecular Weight: 164.20
CAS: 6617-34-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-95.33	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-344.48	kJ/mol	Joback Method
$\Delta_{fus} H°$	10.45	kJ/mol	Joback Method
$\Delta_{vap} H°$	45.84	kJ/mol	Joback Method
$logP_{oct/wat}$	1.36		Crippen Method
P_c	3121.00	kPa	Joback Method
T_{boil}	581.30	K	Joback Method
T_c	822.92	K	Joback Method
T_{fus}	404.20	K	Joback Method
V_c	0.50	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	335.42	J/mol×K	581.3	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O2/c1-5-4-6(11)7-8(9(5)12)10(7,2)3/h4,7-8H,1-3H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).