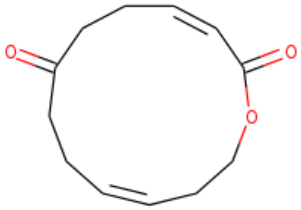
(3E,10Z)-Oxacyclotrideca-3,10-diene-2,7-dione

InChI: InChI=1S/C12H16O3/c13-11-7-3-1-2-6-10-15-12(14)9-5-4-8-11/h1-2,5,9H,3-4,6-8,10H2/b2-1-,9-5+
InChI Key: QPFMJNUWOHGONF-RLKBUKNLSA-N
Formula: C12H16O3
SMILES: O=C1C=CCCC(=O)CCC=CCCO1
Molecular Weight: 208.25
CAS: 144403-15-6



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-273.76	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-551.31	kJ/mol	Joback Method
$\Delta_{fus} H°$	12.34	kJ/mol	Joback Method
$\Delta_{vap} H°$	57.84	kJ/mol	Joback Method
$logP_{oct/wat}$	2.18		Crippen Method
P_c	3005.73	kPa	Joback Method
T_{boil}	688.98	K	Joback Method
T_c	967.11	K	Joback Method
T_{fus}	376.51	K	Joback Method
V_c	0.59	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	477.44	J/mol×K	688.98	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16O3/c13-11-7-3-1-2-6-10-15-12(14)9-5-4-8-11/h1-2,5,9H,3-4,6-8,10H2/b2-1-,9-5+

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).