

# Kinetic data

The most important characteristic of a polymerization initiator is its rate of decomposition expressed by its half-life ( $t_{1/2}$ ). The half-life is the time required to reduce the original amount of peroxide at a given temperature by 50%.



With the exception of hydroperoxides, the half-life is determined by differential scanning calorimetry-thermal activity monitoring (DSC-TAM) of a dilute solution of the initiator in monochloro-benzene. Kinetic data of the decomposition of hydroperoxides in monochloro-benzene are determined titrimetrically.

The tables in this catalog list the temperatures at which the half-lives are 0.1 hour, 1.0 hour and 10 hours.

The half-life can be calculated from the Arrhenius equation

$$k_d = A \cdot e^{-E_a/RT} \text{ and } t_{1/2} = \ln 2/k_d$$

The Arrhenius frequency factor (A) and activation energy ( $E_a$ ) are given in the tables on pages 12-29.

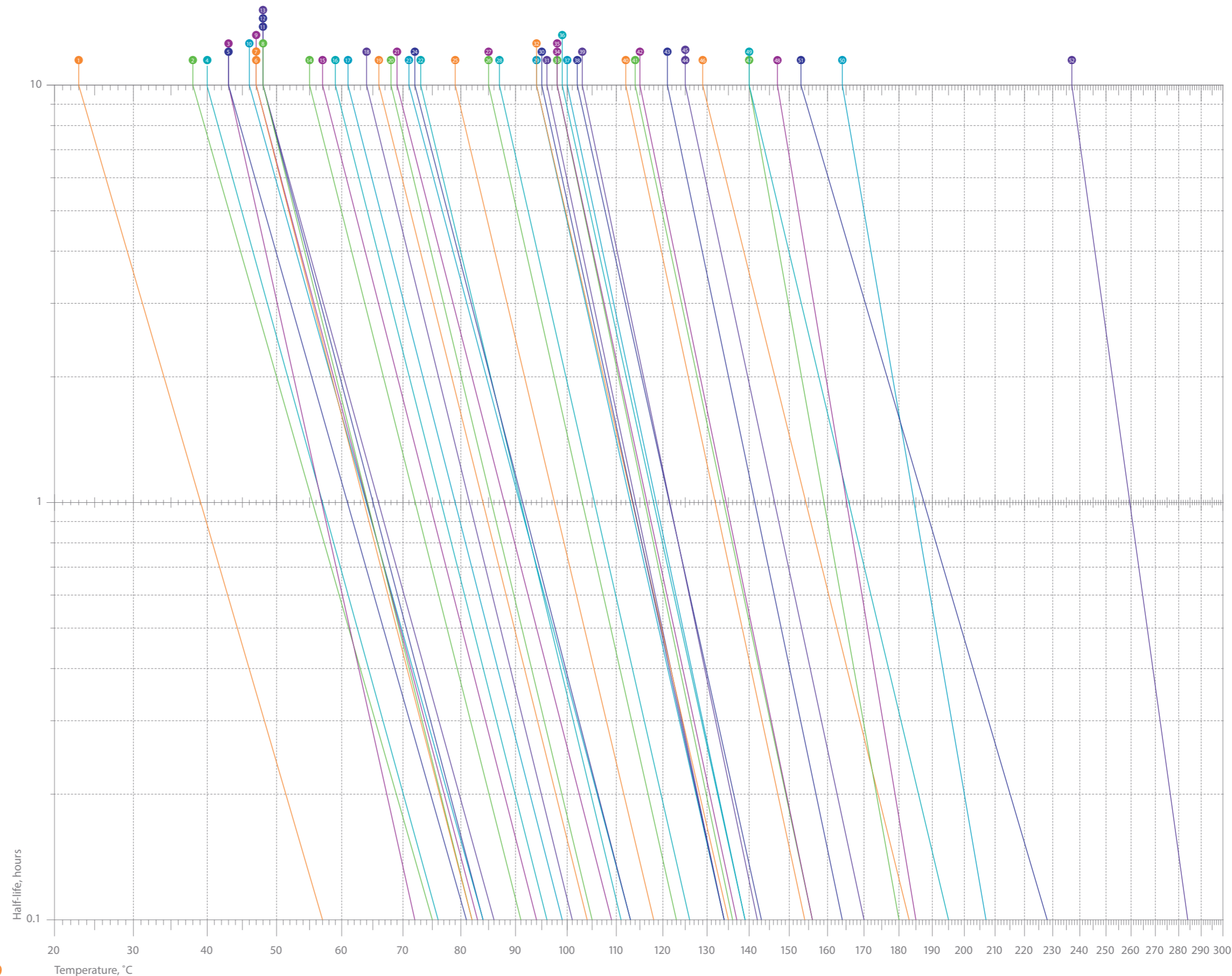
The residual concentration of the initiator can be calculated by means of the equation

$$[I] = [I_0] \cdot e^{-k_d t}$$

The initiators in the tables on pages 12-29 are arranged in descending order of activity, based on the 1.0 hour half-life temperature.

$k_d$  = rate constant for the initiator dissociation in  $s^{-1}$   
 A = Arrhenius frequency factor in  $s^{-1}$   
 $E_a$  = Activation energy for the initiator dissociation in J/mole  
 R = 8.3142 J/mole.K  
 T = temperature in K  
 $t_{1/2}$  = half-life in s  
 $[I_0]$  = original initiator concentration  
 $[I]$  = initiator concentration at time t  
 t = time measured from the start of decomposition in s

# Half-life chart



PRODUCT NAME	CHEMICAL NAME
1 TRIGONOX 187	Diisobutyl peroxide
2 TRIGONOX 99	Cumyl peroxyneodecanoate
3 TRIGONOX 181	Di(3-methoxybutyl) peroxydicarbonate
4 TRIGONOX 423	1,1,3,3-Tetramethylbutyl peroxyneodecanoate
5 TRIGONOX 123	tert-Amyl peroxyneodecanoate
6 TRIGONOX SBP	Di-sec-butyl peroxydicarbonate
7 PERKADOX IPP	Diisopropyl peroxydicarbonate
8 PERKADOX 16	Di(4-tert-butylcyclohexyl) peroxydicarbonate
9 TRIGONOX EHP	Di(2-ethylhexyl) peroxydicarbonate
10 TRIGONOX 23	tert-Butyl peroxyneodecanoate
11 PERKADOX 24	Dicetyl peroxydicarbonate
12 PERKADOX 26	Dimyristyl peroxydicarbonate
13 TRIGONOX 425	1,1,3,3-Tetramethylbutyl peroxy-pivalate
14 TRIGONOX 125	tert-Amyl peroxy-pivalate
15 TRIGONOX 25	tert-Butyl peroxy-pivalate
16 TRIGONOX 36	Di(3,5,5-trimethylhexanoyl) peroxide
17 LAUROX	Dilauroyl peroxide
18 PERKADOX AIBN	2,2'-Azodi(isobutyronitrile)
19 PERKADOX AMBN	2,2'-Azodi(2-methylbutyronitrile)
20 TRIGONOX 141	2,5-Dimethyl-2,5-di(2-ethylhexanoylperoxy)hexane
21 TRIGONOX 421	1,1,3,3-Tetramethylbutyl peroxy-2-ethylhexanoate
22 TRIGONOX 121	tert-Amyl peroxy-2-ethylhexanoate
23 PERKADOX L / CH	Dibenzoyl peroxide
24 TRIGONOX 21	tert-Butyl peroxy-2-ethylhexanoate
25 TRIGONOX 41	tert-Butyl peroxyisobutyrate
26 PERKADOX ACCN	1,1'-Azodi(hexahydrobenzotriazole)
27 TRIGONOX 29	1,1-Di(tert-butylperoxy)-3,3,5-trimethylcyclohexane
28 TRIGONOX 122	1,1-Di(tert-amylperoxy)cyclohexane
29 TRIGONOX 22	1,1-Di(tert-butylperoxy)cyclohexane
30 TRIGONOX 131	tert-Amylperoxy 2-ethylhexyl carbonate
31 TRIGONOX 133	tert-Amyl peroxyacetate
32 TRIGONOX 42	tert-Butyl peroxy-3,5,5-trimethylhexanoate
33 TRIGONOX D	2,2-Di(tert-butylperoxy)butane
34 TRIGONOX BPIC	tert-Butylperoxy isopropyl carbonate
35 TRIGONOX 117	tert-Butylperoxy 2-ethylhexyl carbonate
36 TRIGONOX 127	tert-Amyl peroxybenzoate
37 TRIGONOX F	tert-Butyl peroxyacetate
38 TRIGONOX 17	Butyl 4,4-di(tert-butylperoxy)valerate
39 TRIGONOX C	tert-Butyl peroxybenzoate
40 PERKADOX BC	Dicumyl peroxide
41 PERKADOX 14	Di(tert-butylperoxyisopropyl)benzene(s)
42 TRIGONOX 101	2,5-Dimethyl-2,5-di(tert-butylperoxy)hexane
43 TRIGONOX B	Di-tert-butyl peroxide
44 TRIGONOX 301	3,6,9-Triethyl-3,6,9-trimethyl-1,4,7-triperoxonane
45 TRIGONOX 501	1,2,4,5,7,8-Hexoxonane, 3,6,9-trimethyl-3,6,9-tris(Et and Pr)
46 TRIGONOX M	Isopropylcumyl hydroperoxide
47 TRIGONOX TMBH	1,1,3,3-Tetramethylbutyl hydroperoxide
48 TRIGONOX 311	3,3,5,7,7-Pentamethyl-1,2,4-trioxepane
49 TRIGONOX K	Cumyl hydroperoxide
50 TRIGONOX A	tert-Butyl hydroperoxide
51 TRIGONOX TAHF	tert-Amyl hydroperoxide
52 PERKADOX 30	2,3-Dimethyl-2,3-diphenylbutane