Pentaerythritol tetrakis[3-(3',5'-di-tert-butyl-4'-hydroxyphenyl)pro

Other names:

ADK Stab AO 60

AO 60

Anox 20

Anox 20AM

BP 101

Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,1'-[2,2-bis[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-1,3-pro

Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2,2-bis[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-1,3-propane ester

Dovernox 10

Fenozan 22

Fenozan 23

Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, neopentanetetrayl ester

Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, tetraester with pentaerythritol

IR 1010

Irganox 1010FF

Irganox 1040

Lowinox PP35

MARK AO 60

Naugard 10

Neopentanetetrayl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate

Pentaerythritol, tetrakis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate)

Pentaerythrityl tetrakis-3-(3',5'-di-t-butyl-4'-hydroxyphenyl)propionate

Phenosane 23

RA 1010

Ralox 630

Sumilizer BP 101

Tetraalkofen BPE

Tetrakis [methylene (3,5-di-t-butyl-4-hydroxyhydrocinnamate)] methane

Tetrakis(3,5-di-tert-butyl-4-hydroxyhydrocinnamoyloxymethyl)methane

Tetrakis[methylene(3,5-di-tert-butyl-4-hydroxyhydrocinnamate)methane]

irganox 1010

pentaerythritol tetra(3,5-di-tert-butyl-4-hydroxyhydrocinnamate)

pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate)

tetrakis[methylene-3-(3,5-di-tert-butyl-4-hydroxyphenylpropionate]methane

Inchi: InChI=1S/C73H108O12/c1-65(2,3)49-33-45(34-50(61(49)78)66(4,5)6)25-29-57(74)82-41

InchiKey: BGYHLZZASRKEJE-UHFFFAOYSA-N

Formula: C73H108O12

SMILES: CC(C)(C)c1cc(CCC(=O)OCC(COC(=O)CCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)(COC(=O)

Mol. weight [g/mol]: 1177.63

CAS: 6683-19-8

Physical Properties

Property code	Value	Unit	Source
gf	-592.22	kJ/mol	Joback Method
hf	-2462.88	kJ/mol	Joback Method
hfus	65.95	kJ/mol	Measurement and correlation of solid-liquid equilibria of Irganox 1010 with n-hexane
hfus	65.95	kJ/mol	Solubility of antioxidant 1010 in pure alkanols
hvap	269.51	kJ/mol	Joback Method
log10ws	-17.31		Crippen Method
logp	15.879		Crippen Method
mcvol	997.630	ml/mol	McGowan Method
pc	271.32	kPa	Joback Method
tb	2614.77	K	Joback Method
tc	10442.39	K	Joback Method
tf	1875.61	K	Joback Method
vc	3.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	11392.06	J/mol×K	2614.77	Joback Method
cpg	887201.04	J/mol×K	9137.79	Joback Method
cpg	525485.38	J/mol×K	7833.19	Joback Method
cpg	279487.68	J/mol×K	6528.58	Joback Method
cpg	126766.92	J/mol×K	5223.98	Joback Method
cpg	44882.05	J/mol×K	3919.37	Joback Method
cpg	1387075.69	J/mol×K	10442.39	Joback Method
dvisc	0.0000000	Pa×s	2614.77	Joback Method
dvisc	0.0000000	Pa×s	2491.58	Joback Method
dvisc	0.0000000	Pa×s	2368.38	Joback Method
dvisc	0.0000000	Pa×s	2245.19	Joback Method
dvisc	0.0000000	Pa×s	2122.00	Joback Method
dvisc	0.0000000	Pa×s	1998.80	Joback Method
dvisc	0.0000000	Pa×s	1875.61	Joback Method

Sources

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=C6683198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of antioxidant 1010 in pure alkanols:	https://www.doi.org/10.1016/j.fluid.2008.11.005
Measurement and correlation of solid-liquid equilibria of Irganox 1010 with n-hexane:	https://www.doi.org/10.1016/j.fluid.2009.09.013
Solubility of Irganox 1010 in (Alcohol + Water) Mixtures from (293.15 to 333.15) K:	https://www.doi.org/10.1021/je900435t

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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