

Synonyms:

5,5,6b-trimethyl-3a,4,5,6,6a,6b-hexahydrocyclopropa[e]indene-1a,2(1H)-dicarbaldehyde (ACD/Name)

{Cycloprop[e]indene-1a,2(1H)-dicarboxaldehyde,} 3a,4,5,6,6a, 6b-hexahydro-5,5,6b-trimethyl-, (1a.alpha.,3a.beta.,6a.beta.)

Isovelleral

ISOVELLERAL

CAS: 37841-91-1

NSC: 299922

Formula: C15H20O2

Rings: 3

Atoms: 37

Weight: 232.318

H-Donors: 0

H-Acceptors: 2

Rotatable bonds: 2

Smiles: C1(C[C@H]2[C@@H](C1)C=C([C@]1([C@@]2(C1)))

Toxicity:

Celline	Tox Value	Tox Type
EKVX	4	nlog(LC50)
NCI/ADR-RES	4	nlog(LC50)
CCRF-CEM	4	nlog(LC50)
HL-60(TB)	4	nlog(LC50)
SR	4	nlog(LC50)
T-47D	4.015	nlog(LC50)
OVCAR-8	4.145	nlog(LC50)
A549/ATCC	4.167	nlog(LC50)
SNB-19	4.255	nlog(LC50)
NCI-H322M	4.296	nlog(LC50)
SF-295	4.311	nlog(LC50)
MCF7	4.319	nlog(LC50)
KM12	4.323	nlog(LC50)
HCC-2998	4.345	nlog(LC50)
UACC-62	4.359	nlog(LC50)
RPMI-8226	4.362	nlog(LC50)
HOP-62	4.373	nlog(LC50)
DU-145	4.375	nlog(LC50)
Hs 578T	4.386	nlog(LC50)
MDA-N	4.39	nlog(LC50)
SK-OV-3	4.395	nlog(LC50)
NCI-H460	4.487	nlog(LC50)
UACC-257	4.516	nlog(LC50)
SNB-75	4.532	nlog(LC50)
SN12C	4.573	nlog(LC50)
HCT-15	4.594	nlog(LC50)
K-562	4.619	nlog(LC50)
MOLT-4	4.628	nlog(LC50)
HT29	4.69	nlog(LC50)
NCI-H226	4.698	nlog(LC50)
U251	4.753	nlog(LC50)
M14	4.817	nlog(LC50)
TK-10	4.865	nlog(LC50)
PC-3	4.88	nlog(LC50)
SK-MEL-28	4.96	nlog(LC50)
IGROV1	4.968	nlog(LC50)

NCI-H23	4.994	nlog(LC50)
SK-MEL-2	5.02	nlog(LC50)
OVCAR-5	5.021	nlog(LC50)
CAKI-1	5.052	nlog(LC50)
HOP-92	5.091	nlog(LC50)
MDA-MB-231/ATCC	5.105	nlog(LC50)
SF-268	5.108	nlog(LC50)
SK-MEL-5	5.123	nlog(LC50)
MDA-MB-435	5.167	nlog(LC50)
SW-620	5.176	nlog(LC50)
COLO 205	5.18	nlog(LC50)
786-0	5.191	nlog(LC50)
UO-31	5.193	nlog(LC50)
NCI-H522	5.194	nlog(LC50)
SF-539	5.198	nlog(LC50)
BT-549	5.202	nlog(LC50)
RXF 393	5.223	nlog(LC50)
OVCAR-4	5.225	nlog(LC50)
LOX IMVI	5.23	nlog(LC50)
ACHN	5.269	nlog(LC50)
OVCAR-3	5.286	nlog(LC50)
HCT-116	5.302	nlog(LC50)