

QSAR Applicability Domain (AD) assessment

Substance: CAS 2466-73-1 (isobutyl dihydrogen phosphate)

According to QSAR Applicability Domain (AD) assessment the **fully documented and REACH compliant QSAR** reports are available for following endpoints for the substance **CAS 2466-73-1 (isobutyl dihydrogen phosphate)**:

REACH	OECD	Endpoint	QSAR	AD
Annex VII				
B.1 tris	423	Acute Oral Toxicity	4.2	"near AD limit"
C.3	201	Acute toxicity on algae	3.2	"near AD limit"
C.4	301	Biodegradability	2.3.a	"near AD limit"
C.24	308	Biodegradability in sediment	2.3.a	"in AD"
C.23	307	Biodegradability in soil	2.3.a	"in AD"
	309	Biodegradability in water	2.3.c	"near AD limit"
B.5	405	In vivo Eye Irritation	4.9	"in AD"
C.2	202	Short-term Toxicity testing on Invertebrates	3.1	"in AD"
B.42	429	Skin Sensitisation	4.6	"near AD limit"
B.6	406	Skin Sensitisation	4.6	"in AD"
Annex VIII				
		Abiotic degradation	2.2.b	"near AD limit"
C.11	209	Activated Sludge Respiration Inhibition	3.6	"in AD"
B.2	403	Acute Inhalation Toxicity	4.1	"near AD limit"
C.1	203	Acute toxicity for fish	3.3	"in AD"
	223	Acute Toxicity to Birds	3.12.a	"near AD limit"

C.19	121	Adsorption/Desorption Screening	2.6	"in AD"
B.10	473	Mutagenicity	4.10	"in AD"
B.36	417	Toxicokinetic Behaviour	6.4	"in AD"
Annex IX				
C.13	305	Bioaccumulation in Aquatic Species	2.4a	"in AD"
B.31	414	Prenatal developmental toxicity	4.16	"in AD"
C.17	214	Short-term Toxicity to Invertebrates		"near AD limit"
Annex X				
B.32	451	Carcinogenicity	4.12	"near AD limit"
B.30	452	Chronic toxicity	4.14	"near AD limit"
Additional				
B.36	417	Toxicity to Tetrahymena Pyriformis	3.10	"near AD limit"

The final and extended endpoint data for a single compound is provided in QSAR Property Report Format (QPRF) after detailed research and quality control.

The QSAR reports (QPRF which are endpoint and substance specific) from Molcode do not just contain a numeric prediction value. It is an evaluation of the activity/toxicity with comparisons to experimental data (read-across) and possibly based on several models that give consensus results.