

CrossFire Gmelin

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All Chemical Names (ACN)
All Chemical Name Segments (ACNS)
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Reaction Basic Index (BIREA)
Citation Basic Index (BICIT)

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Formula Search Data (FOR)
Element Count (ELC)
Element Symbol (ELS)
Number of Atoms (NA)
Number of Elements (NE)
Substance Identification (IDE)
Alloy Search Field (ALLOY)
CAS Registry Number (RN)
Chemical Name (CN)
Chemical Name Segment (CNS)
Entry Date (ED)
Fragment Gmelin Registry Number (FRAGRN)
Fragment Molecular Formula (FRAGMF)
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Ligand Formula Count (LIGFC)
Ligand Formulas (LIGFO)
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Linear Structure Formula (LSF)
Modification (MODTXT)
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Molecular Weight (MW)
Number of Components (NC)
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Number of Structures (NSTRUC)
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Update Date (UPD)
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Quantum Chemical Calculations (QCC)

Quantum Chemical Calculations (QUAN)

Bibliographic Information (BIB)

DATA and FIELDS from
Bibliographic Information

Citation (CIT)

Author (AU)
 CODEN (CO)
 CODEN (Translation) (COT)
 Journal Title (JT)
 Journal Title (Translation) (JTT)
 Language (LA)
 Language (Translation) (LAT)
 Publication Year (PY)
 Publication Year (Translation) (PYT)
 DOI (DOI)
 ISSN (ISSN)

Citation Number (CNR)

Citation Number (CNR)

Abstract (AB)

Title (TI)
 Abstract (AB)
 Language (ALA)
 Keywords (AB.KW)

Chemical Properties (CHE)

Chemical Behavior (CHB)

Association (ASS)
 Behavior as Acid / Base (ACBS)
 Behavior as Catalyst (CAT)
 Behavior as Inhibitor (BINH)
 Colloid Chemical Behavior (COLL)
 Decomposition (DP)
 Flash Point (FLAP)
 Information on Stability (STAB)
 Polymerization (POLY)
 Solvation /Hydration (SOHY)

Reaction (RX)

Reaction Code (broad) (RX.BCODE)
 Reaction Code (medium) (RX.MCODE)
 Reaction Code (narrow) (RX.NCODE)
 Reaction ID (RX.ID)
 Reactant(s) (GRN) (RX.RGRN)
 Reactant(s) (Name) (RX.RCT)
 Product(s) (GRN) (RX.PGRN)
 Product(s) (Name) (RX.PRO)
 Number of Details (RX.NVAR)

Reaction Details (RX)

Index Reagents/Catalysts/Solvents (RX.RCS)
 Yield (Numeric) (RX.NYD)
 Yield (RX.YD)
 Reagent (RX.RGT)
 Intermediate(s) (GRN) (RX.IGRN)
 Intermediate(s) (Name) (RX.INT)
 Byproduct (RX.BPRO)
 Solvent (RX.SOL)
 Catalyst(s) (GRN) (RX.CGRN)

Ligand Formulas of one Center (LIG.LIGF0)

Ligand Molecular Formula of one Center
(LIG.LIGMF)

Composition (CMPS)

Percentage (PERC)

Percentage Type (PERT)

Mechanical Properties (MEC)

Compressibility (COMP)

Density (DEN)

Elastic Behavior (ELAS)

Hardness (HARD)

Mole Volume (VOL)

Plastic Behavior (PLAS)

Strength (STRE)

Molecular Properties (MOL)

Bond Dissociation Energy (EDIS)

Conformation and Bonding Models (CONF)

Dipole Moment (DM)

Electronic States (EST)

Intramolecular Distances and Angles
(IDA)

Ionization Potential (IP)

Molecular Rotation (MRC)

Molecular Vibration (VIB)

Polarizability (ELP)

Potential Energy Function (PEF)

Symmetry/Point Group (PGR)

Optical Properties (OPT)

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Electrooptical Effects (ELOP)

Magnetooptical Effects (MAGO)

Optical Anisotropy (OA)

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Melting Gibbs Energy (GFUS)

Sublimation Gibbs Energy (GSUB)

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Boiling Gibbs Energy (GVAP)

Phosphorescence Spectroscopy (PHO)

Raman Spectroscopy (RAS)

Rotational Spectroscopy (ROT)

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(continued in next column)

X-Ray Photoelectron Spectroscopy (XPS)

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Thermodynamic Data (TDD)

Acentric Factor (ACEN)

Cp (Further Information) (CPFI)

Cv (Further Information) (CVFI)

Enthalpy of Formation (Further
Information) (HFFI)

Enthalpy of Formation (HFOR)

Entropy of Formation (Further
Information) (SFFI)

Entropy of Formation (SFOR)

Equation of State (EQST)

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Information)(GFFI)

Gibbs Energy of Formation (GFOR)

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Thermal Conductivity (TCND)

Thermal Expansion (TEC)

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Industrial Synthesis (RX.IND)
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General Conditions (RX.GCON)
Purification/Isolation (RX.ISOL)
Kinetics (RX.KIN)
Update Date (RX.UPD)

**Reaction with Substance
Classes (RCLA)**

Does not React (RCLA.NOREAC)
Does React (RCLA.REAC)
Reaction Product (RCLA.PRO)
Reaction with (RCLA.CL)
Surface Reaction (SURF)