



www.parchem.com

Typical Product Specifications & Properties

(E)-(±)-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one

CAS Number: : 30685-95-1

Specifications	Limits
InChIKey	1S/C13H20O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h6-8,12H,5,9H2,1-4H3/b8-7+
Henry's Law Constant	1.81E-04 atm-m ³ /mole
Water solubility	1.00E+06 mg/L
log P (octanol-water)	3.85
Atmospheric OH Rate Constant	1.43E-10 cm ³ /molecule-sec
Melting Point	< 25 ° C
Molecular weight	192.30
SMILES	C1([C@@H](C(=CCC1)C)\C=C\C(C)=O)(C)C
InChI	UZFLPKAIBPNCA-BQYQJAHWSA-N

