Boron, difluoro(2,4-pentanedionato-O,O')-, (T-4)-

Other names: Boron, difluoro(2,4-pentanedionato)-
Difluoro-2,4-pentanedionatoboron
Boron, difluoro-(pentan-2,4-dionato)-
Boron, difluoro(2,4-pentanedionato-O,O')-
(Acetylacetonato)difluoroboron

Inchi: InChI=1S/C5H7BF2O2/c1-4-3-5(2)10-6(7,8)9-4/h3H,1-2H3

InchiKey: UAEGSWGMLVSQPF-UHFFFAOYSA-N

Formula: C5H7BF2O2

SMILES: CC1=CC(C)=[O+][B-](F)(F)O1

Mol. weight [g/mol]: 147.92

CAS: 15390-25-7

Physical Properties

Property code	Value	Unit	Source
ie	9.20	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
log10ws	0.41		Crippen Method
logp	1.420		Crippen Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15390257&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient