1-(2-Furyl)-4,4,4-trifluoro-1,3-butanedione

Other names:	4,4,4-Trifluoro-1-(2-furyl)-1,3-butanedione
	2-Furoyltrifluoroacetone
	1,3-Butanedione, 4,4,4-trifluoro-1-(2-furanyl)-
	Furonyltrifluoroacetone
	Furoyltrifluoroacetone
	Perfluoroacetyl(2-furoyl)methane
	1,3-Butanedione, 4,4,4-trifluoro-1-(2-furyl)-
	4,4,4-Trifluoro-1-furan-2-yl-butane-1,3-dione
	2-(1,3-Dioxo-4,4,4-trifluorobutyl)furan
	4,4,4-Trifluoro-1-(2-furanyl)-1,3-butanedione
	NSC 9186
	4,4,4-trifluoro-1-(2-furyl)butane-1,3-dione
	4,4,4-Trifluoro-1-(2-furanyl)-butane-1,3-dione
Inchi:	InChI=1S/C8H5F3O3/c9-8(10,11)7(13)4-5(12)6-2-1-3-14-6/h1-3H,4H2
InchiKey:	OWLPCALGCHDBCN-UHFFFAOYSA-N
Formula:	C8H5F3O3
SMILES:	O=C(CC(=O)C(F)(F)F)c1ccco1
Mol. weight [g/mol]:	206.12
CAS:	326-90-9

Physical Properties

Property code	Value	Unit	Source
hsub	70.00 ± 10.00	kJ/mol	NIST Webbook
log10ws	-6.65		Crippen Method
logp	1.984		Crippen Method
mcvol	118.440	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C326909&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume