

Diethyl 2-phthalimidomalonate

Other names:	Diethyl phthalimidomalonate Propanedioic acid, (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-, diethyl ester Ethyl phthalimidomalonate 2-Isoindolinemalonic acid, 1,3-dioxo-, diethyl ester
Inchi:	InChI=1S/C15H15NO6/c1-3-21-14(19)11(15(20)22-4-2)16-12(17)9-7-5-6-8-10(9)13(16)1
InchiKey:	SZNGBHWKVWEBKW-UHFFFAOYSA-N
Formula:	C15H15NO6
SMILES:	CCOC(=O)C(C(=O)OCC)N1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	305.28
CAS:	5680-61-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	0.777		Crippen Method
mcvol	215.590	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5680615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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