N-cyanomethyl phthalimide

Inchi: InChI=1S/C10H6N2O2/c11-5-6-12-9(13)7-3-1-2-4-8(7)10(12)14/h1-4H,6H2
InchiKey: KJTIDLYAIIARFO-UHFFFAOYSA-N
Formula: C10H6N2O2
SMILES: N#CCN1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 186.17
CAS: 3842-20-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	0.806		Crippen Method
mcvol	131.640	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3842204&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