Butanoic acid, morpholide

Other names:	4-Butyrylmorpholine
	Butanoic acid, morpholide
	Morpholine, 4-(1-oxobutyl)-
Inchi:	InChI=1S/C8H15NO2/c1-2-3-8(10)9-4-6-11-7-5-9/h2-7H2,1H3
InchiKey:	BTYJJZJDSMHJGD-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCCC(=O)N1CCOCC1
Mol. weight [g/mol]:	157.21

Physical Properties

Property code	Value	Unit	Source
log10ws	0.60		Cheméo Relay (1.0)
logp	0.645		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
rinpol	1315.00		NIST Webbook
tf	276.57	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5327515&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point