

Imidazole, 5-(n-butylthio)-4-nitro-

Inchi:	InChI=1S/C7H11N3O2S/c1-2-3-4-13-7-6(10(11)12)8-5-9-7/h5H,2-4H2,1H3,(H,8,9)
InchiKey:	HXGNEKDEEFUDGH-UHFFFAOYSA-N
Formula:	C7H11N3O2S
SMILES:	CCCCSc1[nH]cnc1[N+](=O)[O-]
Mol. weight [g/mol]:	201.25
CAS:	116155-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	1.728		Crippen Method
mcvol	143.760	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=C116155023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/14-389-5/Imidazole-5-n-butylthio-4-nitro.pdf>

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