

2-n-Butyl furan

Other names:	2-Butylfuran Furan, 2-butyl-
Inchi:	InChI=1S/C8H12O/c1-2-3-5-8-6-4-7-9-8/h4,6-7H,2-3,5H2,1H3
InchiKey:	NWZIYQNUCXUJJJ-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CCCCc1ccco1
Mol. weight [g/mol]:	124.18
CAS:	4466-24-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	2.622		Crippen Method
mccvol	109.990	ml/mol	McGowan Method
rinpol	894.00		NIST Webbook
rinpol	892.10		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	885.00		NIST Webbook

ripol	882.00	NIST Webbook
ripol	885.00	NIST Webbook
ripol	881.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1119.00	NIST Webbook
ripol	1122.00	NIST Webbook
ripol	1088.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1112.00	NIST Webbook
ripol	1122.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1122.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1130.00	NIST Webbook
ripol	1123.00	NIST Webbook
ripol	1140.00	NIST Webbook
ripol	1138.00	NIST Webbook
ripol	1088.00	NIST Webbook

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=C4466244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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