

Furan, 2-propyl-

Other names:	2-Propylfuran 2-n-Propylfuran Furan, «alpha»-propyl- Furan, Å«alphaÅ»-propyl-
Inchi:	InChI=1S/C7H10O/c1-2-4-7-5-3-6-8-7/h3,5-6H,2,4H2,1H3
InchiKey:	CPLJMYOQYRCCBY-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	CCCC1CCCO1
Mol. weight [g/mol]:	110.15
CAS:	4229-91-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	2.232		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
rinpol	787.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	798.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	781.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	793.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	781.00		NIST Webbook
ripol	1024.00		NIST Webbook
ripol	1027.00		NIST Webbook

ripol	1020.00	NIST Webbook
ripol	1043.00	NIST Webbook
ripol	1011.00	NIST Webbook
ripol	1043.00	NIST Webbook
ripol	1011.00	NIST Webbook
ripol	1033.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47023e+01
Coeff. B	-3.43708e+03
Coeff. C	-4.87780e+01
Temperature range (K), min.	287.22
Temperature range (K), max.	414.78

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4229918&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap:	Vapor pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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