

2-(1-propenyl)furan

Other names:	2-(1-propenyl)furan
Inchi:	InChI=1S/C7H8O/c1-2-4-7-5-3-6-8-7/h2-6H,1H3
InchiKey:	IGWQTPINFQSICW-DUXPYHPUSA-N
Formula:	C7H8O
SMILES:	CC=Cc1ccco1
Mol. weight [g/mol]:	108.14
CAS:	10599-55-0

Physical Properties

Property code	Value	Unit	Source
af	0.2961		Cheméo Relay (1.0)
hf	-0.92	kJ/mol	Cheméo Relay (1.0)
hvap	43.80	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
log10ws	-1.76		Cheméo Relay (1.0)
logp	2.313		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	4231.80	kPa	Cheméo Relay (1.0, beta)
tb	399.59	K	Cheméo Relay (1.0)
tc	605.86	K	Cheméo Relay (1.0)
tf	220.98	K	Cheméo Relay (1.0)
vc	0.340	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C10599550&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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