

2-VINYLFURAN

Other names:	2-Ethenylfuran Furan, 2-ethenyl- Furylethylene
Inchi:	InChI=1S/C6H6O/c1-2-6-4-3-5-7-6/h2-5H,1H2
InchiKey:	QQBUHYQVKJQAOB-UHFFFAOYSA-N
Formula:	C6H6O
SMILES:	C=Cc1ccco1
Mol. weight [g/mol]:	94.11

Physical Properties

Property code	Value	Unit	Source
af	0.2933		Cheméo Relay (1.0)
hf	28.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-10.00 ± 3.00	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	38.00 ± 1.00	kJ/mol	NIST Webbook
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-1.12		Cheméo Relay (1.0)
logp	1.923		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
pc	4648.57	kPa	Cheméo Relay (1.0, beta)
rinpol	761.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	713.00		NIST Webbook
rinpol	721.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	710.00		NIST Webbook
rinpol	725.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1051.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1048.00		NIST Webbook
ripol	1051.00		NIST Webbook

ripol	1051.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1053.00		NIST Webbook
ripol	1054.00		NIST Webbook
ripol	1058.00		NIST Webbook
ripol	1090.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1063.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1085.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1058.00		NIST Webbook
tb	372.65 ± 2.00	K	NIST Webbook
tb	372.00 ± 4.00	K	NIST Webbook
tb	372.95 ± 1.50	K	NIST Webbook
tb	372.70	K	NIST Webbook
tc	582.95	K	Cheméo Relay (1.0)
tf	179.15 ± 4.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	292.20	K	2.30	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1487189&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

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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