

FURAN, 2-(1-PENTENYL)-, (E)-

Other names:	2-[(1E)-1-Pentenyl]furan trans-2-(1-Pentenyl)furan 2-(1-Pentenyl)furan, trans-
Inchi:	InChI=1S/C9H12O/c1-2-3-4-6-9-7-5-8-10-9/h4-8H,2-3H2,1H3/b6-4-
InchiKey:	LKSYSJTUBQSZBS-GQCTYLIASA-N
Formula:	C9H12O
SMILES:	CCC/C=C/c1ccco1
Mol. weight [g/mol]:	136.19

Physical Properties

Property code	Value	Unit	Source
af	0.3451		Cheméo Relay (1.0)
hf	-52.46	kJ/mol	Cheméo Relay (1.0)
hvap	48.68	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
log10ws	-3.19		Cheméo Relay (1.0)
logp	3.093		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3190.07	kPa	Cheméo Relay (1.0, beta)
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
tb	450.41	K	Cheméo Relay (1.0)
tc	636.50	K	Cheméo Relay (1.0)
tf	207.67	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20992692&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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