3-(2-furyl)-2-propenal

Other names:	1-(2-furanyl)-1-propen-3-al
	2-Furanacrolein
	3-(2-Furanyl)-2-propenal
	3-(2-Furyl)acrolein
	3-(2-furyl)acrylaldehyde
	3-(«alpha»-Furyl)propenal
	NSC 2061
	NSC 26338
	«beta»-(2-Furyl)acrolein
Inchi:	InChI=1S/C7H6O2/c8-5-1-3-7-4-2-6-9-7/h1-6H
InchiKey:	VZIRCHXYMBFNFD-HNQUOIGGSA-N
Formula:	C7H6O2
SMILES:	O=CC=Cc1ccco1
Mol. weight [g/mol]:	122.12
CAS:	39511-08-5

Physical Properties

Property code	Value	Unit	Source
af	0.3774		Cheméo Relay (1.0)
hf	-125.47	kJ/mol	Cheméo Relay (1.0)
hvap	55.37	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-0.82		Cheméo Relay (1.0)
logp	1.492		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
pc	4987.89	kPa	Cheméo Relay (1.0, beta)
tb	472.40	K	Cheméo Relay (1.0)
tc	685.58	K	Cheméo Relay (1.0)
tf	268.36	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hvapt	82.30	kJ/mol	298.15	Standard molar enthalpies of formation of some vinylfuran derivatives

Sources

Cheméo Relay (1.0, beta):

Standard molar enthalpies of formation of some vinylfuran derivatives: https://www.doi.org/10.1016/j.jct.2008.09.013

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39511085&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

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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