2-Propenal, 3-(2-furanyl)-

Other names:	2-Furanacrolein
	3-(«alpha»-Furyl)propenal
	3-(2-Furyl)acrolein
	3-(2-Furyl)-2-propenal
	«beta»-(2-Furyl)acrolein
	3-(2-Furanyl)-2-propenal
	NSC 2061
	NSC 26338
	1-(2-furanyl)-1-propen-3-al
	3-(2-furyl)acrylaldehyde
Inchi:	InChI=1S/C7H6O2/c8-5-1-3-7-4-2-6-9-7/h1-6H/b3-1+
InchiKey:	VZIRCHXYMBFNFD-HNQUOIGGSA-N
Formula:	C7H6O2
SMILES:	O=CC=Cc1ccco1
Mol. weight [g/mol]:	122.12
CAS:	623-30-3

Physical Properties

Property code	Value	Unit	Source
chs	-3430.00 ± 0.80	kJ/mol	NIST Webbook
hf	-106.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-182.00 ± 0.80	kJ/mol	NIST Webbook
hsub	76.00	kJ/mol	NIST Webbook
log10ws	-5.73		Crippen Method
logp	1.492		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
rinpol	1111.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1831.00		NIST Webbook
ripol	1851.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	76.00 ± 2.00	kJ/mol	289.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623303&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices