2-Furancarboxylic acid, ethyl ester

Other names:	2-Furoic acid, ethyl ester
	Ethyl furan-2-carboxylate
	Ethyl pyromucate
	Ethyl 2-furancarboxylate
	Ethyl 2-furoate
	Furan-2-carboxylic acid ethyl ester
	2-Carboethoxyfuran
	2-(Ethoxycarbonyl)furan
	Ethyl 2-furylcarboxylate
	NSC 2304
	Ethyl furoate
Inchi:	InChI=1S/C7H8O3/c1-2-9-7(8)6-4-3-5-10-6/h3-5H,2H2,1H3
InchiKey:	NHXSTXWKZVAVOQ-UHFFFAOYSA-N
Formula:	C7H8O3
SMILES:	CCOC(=O)c1ccco1
Mol. weight [g/mol]:	140.14
CAS:	614-99-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	1.456		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
rinpol	1074.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1029.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1056.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1611.00		NIST Webbook

ripol	1605.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1606.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1602.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1621.00		NIST Webbook
ripol	1608.00		NIST Webbook
tb	470.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	51.20	kJ/mol	371.50	NIST Webbook
hvapt	52.60	kJ/mol	389.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.20	K	13.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C614993&Units=SI
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

Legend

hvapt:	Enthalpy of vaporization 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure