2-Furancarboxylic acid

Other names:	.alpha.-furancarboxylic acid
	.alpha.-furoic acid
	2-Carboxyfuran
	2-Furanoic acid
	2-Furoic acid
	2-furancarboxilic acid
	Furan-2-carboxylic acid
	Furancarboxylic acid-(2)
	Furoic acid
	Furoica
	Kyselina 2-furoova
	Kyselina pyroslizova
	NSC 8842
	Pyromucic acid
	«alpha»-Furancarboxylic acid
	«alpha»-Furoic acid
	Â«alphaÂ»-Furancarboxylic acid
	Â«alphaÂ»-Furoic acid
Inchi:	InChI=1S/C5H4O3/c6-5(7)4-2-1-3-8-4/h1-3H,(H,6,7)
InchiKey:	SMNDYUVBFMFKNZ-UHFFFAOYSA-N
Formula:	C5H4O3
SMILES:	O=C(O)c1ccco1
Mol. weight [g/mol]:	112.08
CAS:	88-14-2

Physical Properties

Property code	Value	Unit	Source
hsub	88.40 ± 1.50	kJ/mol	NIST Webbook
ie	9.32	eV	NIST Webbook
ie	9.16 ± 0.05	eV	NIST Webbook
ie	9.17	eV	NIST Webbook
log10ws	-0.49		Aqueous Solubility Prediction Method
logp	0.978		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
rinpol	1087.80		NIST Webbook
tb	504.20	K	NIST Webbook

tf	405.15 ± 0.70	K	NIST Webbook
tf	406.65 ± 1.00	K	NIST Webbook
tf	403.55	K	Measurement and Correlation of Solubility and Dissolution Thermodynamic Properties of Furan-2-carboxylic Acid in Pure and Binary Solvents
tf	405.48	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	132.26	J/mol×K	298.15	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins
hfust	22.60	kJ/mol	402.50	NIST Webbook
hsubt	108.40 ± 2.20	kJ/mol	322.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.70	K	2.70	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins:	https://www.doi.org/10.1016/j.tca.2017.06.024

Mutual Influence of Furfural and Furancarboxylic Acids on Their Solubility in Aqueous Solutions: Experiments and Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) Predictions. https://www.doi.org/10.1021/acs.jced.7b01039

Measurement and Correlation of Solubility and Dissolution Thermodynamic Properties of Furan-2-carboxylic Acid in Pure and Binary Solvents: https://www.doi.org/10.1021/je500012b

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point