

2-furoic acid

Other names:	.alpha.-furancarboxylic acid
	.alpha.-furoic acid
	2-Furanoic acid
	2-carboxyfuran
	2-furancarboxilic acid
	2-furancarboxylic acid
	Furan-2-carboxylic acid
	Furancarboxylic acid-(2)
	Furoic acid
	Furoica
	Kyselina 2-furoova
	Kyselina pyroslizova
	NSC 8842
	pyromucic acid
	«alpha»-Furancarboxylic 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:	26447-28-9

Physical Properties

Property code	Value	Unit	Source
chs	-2040.70	kJ/mol	NIST Webbook
hf	-390.50	kJ/mol	NIST Webbook
hf	-395.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-498.48	kJ/mol	NIST Webbook
hfs	-503.00 ± 2.00	kJ/mol	NIST Webbook
hsub	108.00	kJ/mol	NIST Webbook
hsub	108.40 ± 2.40	kJ/mol	NIST Webbook
hvap	72.02	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-0.49		Aqueous Solubility Prediction Method
logp	0.978		Crippen Method

mvol	75.160	ml/mol	McGowan Method
tb	505.26	K	Cheméo Relay (1.0)
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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26447289&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the mutual influence of Furfural and Furan-2-carboxylic Acids on the Solubility of Aqueous Solutions:	https://www.doi.org/10.1016/j.tca.2017.06.024
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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	https://www.doi.org/10.1021/je500012b
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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