3-Thiophenecarboxylic acid

Other names:	.beta.-thiophenecarboxylic acid
	.beta.-thiophenic acid
	3-Thenoic acid
	Thiophene-3-carboxylic acid
	«beta»-Thiophenecarboxylic acid
	«beta»-Thiophenic acid
	Â«betaÂ»-Thiophenecarboxylic acid
	Â«betaÂ»-Thiophenic acid
Inchi:	InChI=1S/C5H4O2S/c6-5(7)4-1-2-8-3-4/h1-3H,(H,6,7)
InchiKey:	YNVOMSDITJMNET-UHFFFAOYSA-N
Formula:	C5H4O2S
SMILES:	O=C(O)c1ccsc1
Mol. weight [g/mol]:	128.15
CAS:	88-13-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Aqueous Solubility Prediction Method
logp	1.446		Crippen Method
mcvol	85.640	ml/mol	McGowan Method
tf	411.65	K	Aqueous Solubility Prediction Method
tf	411.85	K	Solid-liquid equilibrium and thermodynamic research of 3-Thiophenecarboxylic acid in (water + acetic acid) binary solvent mixtures

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	18.30	kJ/mol	412.90	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-liquid equilibrium and thermodynamic research of 3-Thiophenecarboxylic acid in (water + acetic acid) binary solvent mixtures:	https://www.doi.org/10.1016/j.tca.2014.11.008
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=C88131&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point