2,5-Furandicarboxylic acid

Other names:	2,5-dicarboxyfuran
	Dehydromucic acid
	Furan-2,5-dicarboxylic acid
	Furane-«alpha»,«alpha»'-dicarboxylic acid
Inchi:	InChI=1S/C6H4O5/c7-5(8)3-1-2-4(11-3)6(9)10/h1-2H,(H,7,8)(H,9,10)
InchiKey:	CHTHALBTIRVDBM-UHFFFAOYSA-N
Formula:	C6H4O5
SMILES:	O=C(O)c1ccc(C(=O)O)o1
Mol. weight [g/mol]:	156.09
CAS:	3238-40-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	0.676		Crippen Method
mcvol	96.690	ml/mol	McGowan Method
tf	614.45	K	Solubilities of 2,5-Furandicarboxylic Acid in Binary Acetic Acid + Water, Methanol + Water, and Ethanol + Water Solvent Mixtures

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	121.30	kJ/mol	390.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 2,5-Furandicarboxylic Acid in Eight Pure Solvents and Two Binary Solvent Systems at 313.15-363.15 K:	https://www.doi.org/10.1021/acs.jced.7b00927

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
Solubilities of 2,5-Furandicarboxylic Acid in Binary Acetic Acid + Water, Methanol + Water, and Ethanol + Water Solvent Mixtures:	https://www.doi.org/10.1021/acs.jced.7b01112
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3238402&Units=SI

Legend

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
tf:	Normal melting (fusion) point