2-Thienylamide

Other names:	2-(Aminocarbonyl)thiophene
	2-Thenamide
	2-Thiophenecarboxamide
	Thiophene-2-carboxamide
Inchi:	InChI=1S/C5H5NOS/c6-5(7)4-2-1-3-8-4/h1-3H,(H2,6,7)
InchiKey:	DENPQNAWGQXKCU-UHFFFAOYSA-N
Formula:	C5H5NOS
SMILES:	NC(=O)c1cccs1
Mol. weight [g/mol]:	127.16
CAS:	5813-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.40		Crippen Method
logp	0.847		Crippen Method
mcvol	89.750	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhos	1031.00	kg/m3	298.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide:	https://www.doi.org/10.1016/j.jct.2007.07.004

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rhos: Solid Density

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https://www.chemeo.com/cid/98-429-8/2-Thienylamide.pdf

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