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]:	127.17

Physical Properties

Property code	Value	Unit	Source
hf	-113.05	kJ/mol	Cheméo Relay (1.0)
hvap	58.48	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-1.62		Cheméo Relay (1.0)
logp	0.847		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
tb	530.08	K	Cheméo Relay (1.0)
tf	386.44	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5813898&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation 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
rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point