# 2-thiopheneacetamide

Inchi: InChi=1S/C6H7NOS/c7-6(8)4-5-2-1-3-9-5/h1-3H,4H2,(H2,7,8)

InchiKey: UUPZTFTUZUQRQT-UHFFFAOYSA-N

Formula: C6H7NOS

SMILES: NC(=O)Cc1cccs1

**Mol. weight [g/mol]:** 141.20

## **Physical Properties**

Property code	Value	Unit	Source
log10ws	-1.24		Crippen Method
logp	0.776		Crippen Method
mcvol	103.840	ml/mol	McGowan Method

### **Temperature Dependent Properties**

Property code	Value	Unit	Temperature [K	(] Source	
psub	9.80e-05	kPa		Standard molar enthalpies of formation and of sublimation of thiophenecarboxamide and 2-thiopheneacetamide	
psub	9.30e-05	kPa		Standard molar enthalpies of formation and of sublimation of thiophenecarboxamide and 2-thiopheneacetamide	
psub	9.40e-05	kPa		Standard molar enthalpies of formation and of sublimation of thiophenecarboxamide and 2-thiopheneacetamide	

psub	1.17e-04	kPa	336.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.16e-04	kPa	336.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.18e-04	kPa	336.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.49e-04	kPa	338.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.48e-04	kPa	338.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.40e-04	kPa	338.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.78e-04	kPa	340.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.87e-04	kPa	340.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.83e-04	kPa	340.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide

psub	2.32e-04	kPa	342.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	2.31e-04	kPa	342.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	2.28e-04	kPa	342.20	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	2.87e-04	kPa	344.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	2.83e-04	kPa	344.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	2.78e-04	kPa	344.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	3.66e-04	kPa	346.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	3.61e-04	kPa	346.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide

ps	sub	3.50e-04	kPa	346.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	4.49e-04	kPa	348.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	4.33e-04	kPa	348.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	4.30e-04	kPa	348.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	5.48e-04	kPa	350.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	5.33e-04	kPa	350.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	5.32e-04	kPa	350.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	6.71e-04	kPa	352.14	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	
ps	sub	6.73e-04	kPa	352.14	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxami and 2-thiopheneacetamid	

noub 6.50° 04 PD- 050.44	
	Standard molar enthalpies of formation and of sublimation of -thiophenecarboxamide and 2-thiopheneacetamide
	Standard molar enthalpies of formation and of sublimation of -thiophenecarboxamide and 2-thiopheneacetamide
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	Standard molar enthalpies of formation and of sublimation of -thiophenecarboxamide and 2-thiopheneacetamide

#### **Sources**

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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 https://www.doi.org/10.1016/j.jct.2007.07.004 and of sublimation of

2-thiophenecarboxamide and 2-thiopheneacetamide:

#### Legend

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficientmcvol: McGowan's characteristic volume

**psub:** Sublimation pressure

rhos: Solid Density

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