

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	334.12	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	9.30e-05	kPa	334.12	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	9.40e-05	kPa	334.12	Standard molar enthalpies of formation and of sublimation of 2-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

psub	3.50e-04	kPa	346.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	4.49e-04	kPa	348.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	4.33e-04	kPa	348.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	4.30e-04	kPa	348.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	5.48e-04	kPa	350.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	5.33e-04	kPa	350.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	5.32e-04	kPa	350.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	6.71e-04	kPa	352.14	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	6.73e-04	kPa	352.14	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide

psub	6.59e-04	kPa	352.14	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	8.33e-04	kPa	354.18	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	8.28e-04	kPa	354.18	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	8.06e-04	kPa	354.18	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.01e-03	kPa	356.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	1.01e-03	kPa	356.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
psub	9.93e-04	kPa	356.19	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide
rhos	1069.00	kg/m3	298.15	Standard molar enthalpies of formation and of sublimation of 2-thiophenecarboxamide and 2-thiopheneacetamide

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Standard molar enthalpies of formation and of sublimation of <https://www.doi.org/10.1016/j.jct.2007.07.004>

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

2-thiopheneacetamide and Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
rhos:	Solid Density

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