

4-hydroxy-2,5-dimethyl-3(2H)-thiophenone

Other names:	3(2H)-Thiophenone, 4-hydroxy-2,5-dimethyl-4-hydroxy-2,5-dimethylthiophen-3(2H)-one
Inchi:	InChI=1S/C6H8O2S/c1-3-5(7)6(8)4(2)9-3/h3,8H,1-2H3
InchiKey:	LMGFTFOLCQQHHC-UHFFFAOYSA-N
Formula:	C6H8O2S
SMILES:	CC1=C(O)C(=O)C(C)S1
Mol. weight [g/mol]:	144.19
CAS:	26494-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-172.66	kJ/mol	Joback Method
hf	-316.52	kJ/mol	Joback Method
hfus	12.93	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.480		Crippen Method
mcvol	104.030	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
rinpol	1181.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1158.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2040.00		NIST Webbook
tb	568.91	K	Joback Method
tc	788.77	K	Joback Method
tf	406.57	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.49	J/molxK	568.91	Joback Method

cpg	244.21	J/mol×K	605.55	Joback Method
cpg	253.50	J/mol×K	642.20	Joback Method
cpg	262.34	J/mol×K	678.84	Joback Method
cpg	270.72	J/mol×K	715.48	Joback Method
cpg	278.63	J/mol×K	752.13	Joback Method
cpg	286.06	J/mol×K	788.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26494100&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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