

Ethanethioic acid, S-(3-methoxyphenyl) ester

Other names:	3-Methoxythiophenol, S-acetyl- S-(3-Methoxyphenyl) ethanethioate
Inchi:	InChI=1S/C9H10O2S/c1-7(10)12-9-5-3-4-8(6-9)11-2/h3-6H,1-2H3
InchiKey:	BSUMOLODBDMGEB-UHFFFAOYSA-N
Formula:	C9H10O2S
SMILES:	<chem>COc1cccc(SC(C)=O)c1</chem>
Mol. weight [g/mol]:	182.24
CAS:	69746-44-7

Physical Properties

Property code	Value	Unit	Source
gf	-73.12	kJ/mol	Joback Method
hf	-206.96	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.334		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1506.80		NIST Webbook
tb	582.05	K	Joback Method
tc	819.33	K	Joback Method
tf	336.69	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.44	J/molxK	582.05	Joback Method
cpg	315.94	J/molxK	621.60	Joback Method
cpg	327.66	J/molxK	661.14	Joback Method
cpg	338.59	J/molxK	700.69	Joback Method
cpg	348.75	J/molxK	740.23	Joback Method
cpg	358.12	J/molxK	779.78	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=C69746447&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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