4-Methoxycarbonylphenyl isothiocyanate

Inchi:	InChI=1S/C9H7NO2S/c1-12-9(11)7-2-4-8(5-3-7)10-6-13/h2-5H,1H3
InchiKey:	WIZODHILGBTPPA-UHFFFAOYSA-N
Formula:	C9H7NO2S
SMILES:	COC(=O)c1ccc(N=C=S)cc1
Mol. weight [g/mol]:	193.22
CAS:	3662-78-0

Physical Properties

Property code	Value	Unit	Source
hf	35.24	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.208		Crippen Method
mcvol	139.080	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
tb	659.22	K	Joback Method
tc	916.43	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3662780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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