3-Ethylphenyl isothiocyanate

Inchi:	InChI=1S/C9H9NS/c1-2-8-4-3-5-9(6-8)10-7-11/h3-6H,2H2,1H3
InchiKey:	FRMFJQIVPNSSPX-UHFFFAOYSA-N
Formula:	C9H9NS
SMILES:	CCc1cccc(N=C=S)c1
Mol. weight [g/mol]:	163.24
CAS:	19241-20-4

Physical Properties

Property code	Value	Unit	Source
hf	280.04	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.983		Crippen Method
mcvol	131.640	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	582.93	K	Joback Method
tc	837.99	K	Joback Method

Sources

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=C19241204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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