

3,4-Xylyl isothiocyanate

Inchi:	InChI=1S/C9H9NS/c1-7-3-4-9(10-6-11)5-8(7)2/h3-5H,1-2H3
InchiKey:	JFSHJWKBNJMGOK-UHFFFAOYSA-N
Formula:	C9H9NS
SMILES:	Cc1ccc(N=C=S)cc1C
Mol. weight [g/mol]:	163.24
CAS:	19241-17-9

Physical Properties

Property code	Value	Unit	Source
hf	268.57	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.038		Crippen Method
mvol	131.640	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
tb	587.91	K	Joback Method
tc	844.05	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241179&Units=SI
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

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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