

2,6-Dimethylphenyl isothiocyanate

Other names:	Benzene, 2-isothiocyanato-1,3-dimethyl- 2,6-Dimethylphenyl-1-isothiocyanate Isothiocyanic acid, 2,6-xylyl ester 2,6-Xylyl isothiocyanate
Inchi:	InChI=1S/C9H9NS/c1-7-4-3-5-8(2)9(7)10-6-11/h3-5H,1-2H3
InchiKey:	UULUECCNPPJFBU-UHFFFAOYSA-N
Formula:	C9H9NS
SMILES:	<chem>Cc1cccc(C)c1N=C=S</chem>
Mol. weight [g/mol]:	163.24
CAS:	19241-16-8

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
mcvol	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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241168&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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