3-Methylbenzyl isothiocyanate

Inchi: InChI=1S/C9H9NS/c1-8-3-2-4-9(5-8)6-10-7-11/h2-5H,6H2,1H3
InchiKey: NUXFAFWRXGFTQJ-UHFFFAOYSA-N
Formula: C9H9NS
SMILES: Cc1cccc(CN=C=S)c1
Mol. weight [g/mol]: 163.24
CAS: 3696-66-0

Physical Properties

Property code	Value	Unit	Source
hf	280.04	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.598		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=C3696660&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