L-«alpha»-Methylbenzyl isothiocyanate

Inchi: InChI=1S/C9H9NS/c1-8(10-7-11)9-5-3-2-4-6-9/h2-6,8H,1H3/t8-/m1/s1
InchiKey: QQCJPTVZIZVKEZ-MRVPVSSYSA-N
Formula: C9H9NS
SMILES: CC(N=C=S)c1ccccc1
Mol. weight [g/mol]: 163.24
CAS: 24277-43-8

Physical Properties

Property code	Value	Unit	Source
hf	286.23	kJ/mol	Joback Method
hvap	47.96	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.850		Crippen Method
mcvol	131.640	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	577.51	K	Joback Method
tc	837.49	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=C24277438&Units=SI

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