

DL-«alpha»-Methylbenzyl isothiocyanate

Inchi: InChI=1S/C9H9NS/c1-8(10-7-11)9-5-3-2-4-6-9/h2-6,8H,1H3
InchiKey: QQCJPTVZIZVKEZ-UHFFFAOYSA-N
Formula: C9H9NS
SMILES: CC(N=C=S)c1ccccc1
Mol. weight [g/mol]: 163.24
CAS: 32393-32-1

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C32393321&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

Latest version available from:

<https://www.cheméo.com/cid/65-776-9/DL-alpha-Methylbenzyl-isothiocyanate.pdf>

Generated by Cheméo on 2024-04-26 08:01:59.092693955 +0000 UTC m=+16407768.013271271.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.