

3-Methoxybenzylisothiocyanate

Inchi:	InChI=1S/C9H9NOS/c1-11-9-4-2-3-8(5-9)6-10-7-12/h2-5H,6H2,1H3
InchiKey:	SSSDJJXWAVRNCM-UHFFFAOYSA-N
Formula:	C9H9NOS
SMILES:	COc1cccc(CN=C=S)c1
Mol. weight [g/mol]:	179.24
CAS:	75272-77-4

Physical Properties

Property code	Value	Unit	Source
hf	147.82	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.298		Crippen Method
mcpvol	137.510	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1605.00		NIST Webbook
tb	605.35	K	Joback Method
tc	856.17	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75272774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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