4-Methoxybenzyl isothiocyanate

Other names: p-Methoxybenzyl isothiocyanate
Inchi: InChI=1S/C9H9NOS/c1-11-9-4-2-8(3-5-9)6-10-7-12/h2-5H,6H2,1H3
InchiKey: IMFQYAJJXFXVMM-UHFFFAOYSA-N
Formula: C9H9NOS
SMILES: COc1ccc(CN=C=S)cc1
Mol. weight [g/mol]: 179.24
CAS: 3694-57-3

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
mcvol	137.510	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1635.90		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1635.90		NIST Webbook
ripol	2482.00		NIST Webbook
ripol	2482.00		NIST Webbook
tb	605.35	K	Joback Method
tc	856.17	K	Joback Method

Sources

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=C3694573&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature