1-Naphthalenemethyl isothiocyanate

Inchi: InChI=1S/C12H9NS/c14-9-13-8-11-6-3-5-10-4-1-2-7-12(10)11/h1-7H,8H2
InchiKey: JJMDUNWYBZCIKZ-UHFFFAOYSA-N
Formula: C12H9NS
SMILES: S=C=NCc1cccc2ccccc12
Mol. weight [g/mol]: 199.27
CAS: 17112-82-2

Physical Properties

Property code	Value	Unit	Source
hf	409.19	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.443		Crippen Method
mcvol	154.450	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	670.55	K	Joback Method
tc	941.41	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17112822&Units=SI
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

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