cis-Raphasatin

Inchi: InChI=1S/C6H9NS2/c1-9-5-3-2-4-7-6-8/h3,5H,2,4H2,1H3/b5-3-
InchiKey: RYSPJKHYSHFYEB-HYXAFXHYSA-N
Formula: C6H9NS2
SMILES: CSC=CCCN=C=S
Mol. weight [g/mol]: 159.27
CAS: 123954-93-8

Physical Properties

Property code	Value	Unit	Source
hf	275.99	kJ/mol	Joback Method
hvap	46.17	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.356		Crippen Method
mcvol	125.180	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1419.20		NIST Webbook
rinpol	1419.20		NIST Webbook
tb	555.57	K	Joback Method
tc	802.54	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C123954938&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature