

trans-Raphasatin

Inchi: InChI=1S/C6H9NS2/c1-9-5-3-2-4-7-6-8/h3,5H,2,4H2,1H3/b5-3+
InchiKey: RYSPJKHYSHFYEB-HWKANZROSA-N
Formula: C6H9NS2
SMILES: CSC=CCCN=C=S
Mol. weight [g/mol]: 159.27
CAS: 13028-50-7

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	1441.60		NIST Webbook
rinpol	1441.60		NIST Webbook
tb	555.57	K	Joback Method
tc	802.54	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=C13028507&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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