

Lesquerellin

Inchi: InChI=1S/C8H15NS2/c1-11-7-5-3-2-4-6-9-8-10/h2-7H2,1H3
InchiKey: YIBXPFAXPUDDTK-UHFFFAOYSA-N
Formula: C8H15NS2
SMILES: CSCCCCCCN=C=S
Mol. weight [g/mol]: 189.34
CAS: 4430-39-1

Physical Properties

Property code	Value	Unit	Source
hf	117.49	kJ/mol	Joback Method
hvap	50.66	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.013		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	597.17	K	Joback Method
tc	823.75	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=C4430391&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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