Alyssin

Inchi: InChI=1S/C7H13NOS2/c1-11(9)6-4-2-3-5-8-7-10/h2-6H2,1H3
InchiKey: IUUQPVQTAUKPPB-UHFFFAOYSA-N
Formula: C7H13NOS2
SMILES: CS(=O)CCCCCN=C=S
Mol. weight [g/mol]: 191.31
CAS: 646-23-1

Physical Properties

Property code	Value	Unit	Source
hf	-109.48	kJ/mol	Joback Method
hvap	54.34	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.638		Crippen Method
mcvol	149.440	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
tb	563.79	K	Joback Method
tc	780.74	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=C646231&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature