Sulforaphane

Inchi: InChI=1S/C6H11NOS2/c1-10(8)5-3-2-4-7-6-9/h2-5H2,1H3
InchiKey: SUVMJBTUFCVSAD-UHFFFAOYSA-N
Formula: C6H11NOS2
SMILES: CS(=O)CCCCN=C=S
Mol. weight [g/mol]: 177.29
CAS: 4478-93-7

Physical Properties

Property code	Value	Unit	Source
hf	-88.84	kJ/mol	Joback Method
hvap	52.12	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	1.248		Crippen Method
mcvol	135.350	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	540.91	K	Joback Method
tc	761.70	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4478937&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