

6-Ethyl-4,5,7,8-tetrathia-cis-2-undecene

Inchi:	InChI=1S/C9H18S4/c1-4-7-10-12-9(6-3)13-11-8-5-2/h4,7,9H,5-6,8H2,1-3H3/b7-4+
InchiKey:	MMZWJALGNZCSLI-QPJXVBHSA-N
Formula:	C9H18S4
SMILES:	CC=CSSC(CC)SSCCC
Mol. weight [g/mol]:	254.50
CAS:	126876-36-6

Physical Properties

Property code	Value	Unit	Source
gf	235.16	kJ/mol	Joback Method
hf	50.33	kJ/mol	Joback Method
hfus	32.26	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.429		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1813.10		NIST Webbook
rinpol	1755.90		NIST Webbook
rinpol	1755.90		NIST Webbook
tb	684.16	K	Joback Method
tc	936.50	K	Joback Method
tf	308.71	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.10	J/molxK	684.16	Joback Method
cpg	489.15	J/molxK	726.22	Joback Method
cpg	503.06	J/molxK	768.27	Joback Method
cpg	515.85	J/molxK	810.33	Joback Method
cpg	527.53	J/molxK	852.39	Joback Method

cpg	538.11	J/mol×K	894.45	Joback Method
cpg	547.62	J/mol×K	936.50	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=C126876366&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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