4H-1,3-DITHIIN, 4-METHYL-2-(1-PROPENYL)-

Other names: 4-Methyl-2-propenyl-4H-[1,3]dithiine
Inchi: InChI=1S/C8H12S2/c1-3-4-8-9-6-5-7(2)10-8/h3-8H,1-2H3/b4-3+
InchiKey: ALDAFTNRTWJFQH-ONEGZZNKSA-N
Formula: C8H12S2
SMILES: C/C=C/C1SC=CC(C)S1
Mol. weight [g/mol]: 172.32

Physical Properties

Property code	Value	Unit	Source
hfus	18.12	kJ/mol	Joback Method
logp	3.271		Crippen Method
mcvol	136.820	ml/mol	McGowan Method
rinpol	1331.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.26	J/mol×K	496.30	Joback Method
cpg	294.45	J/mol×K	537.15	Joback Method
cpg	309.55	J/mol×K	577.99	Joback Method
cpg	323.60	J/mol×K	618.84	Joback Method
cpg	336.67	J/mol×K	659.69	Joback Method
cpg	348.81	J/mol×K	700.53	Joback Method
cpg	360.07	J/mol×K	741.38	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60051356&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices